ARPES and STM

Methods and their application for Tis characterisation

A. Kaplan, University of Birmingham, UK

Angle-Resolved Photoemission Spectroscopy

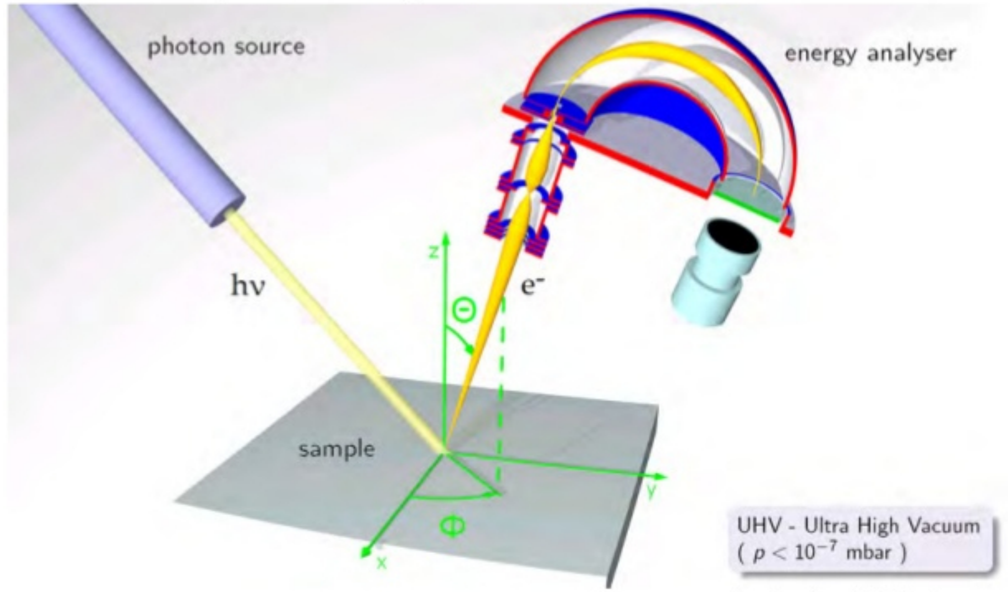
ARPES

- Experiment
- Theory
- Examples

PES Experiment

- rare gas discharge lamp (<40.2 eV)
- x-ray tube (1.256 and 1.486 keV)
- synchrotron radiation (10 eV ... 10 keV)

- hemispherical anylzer
- time of flight (TOF) analyzer)



typically 10^{-10} mbar

Wikipedia

$$K = \frac{\sqrt{2mE_{kin}}}{\hbar}$$

$$\vec{K}_{\parallel} = \vec{K}_x + \vec{K}_y$$

$$\vec{K}_{\perp} = \vec{K}_z$$

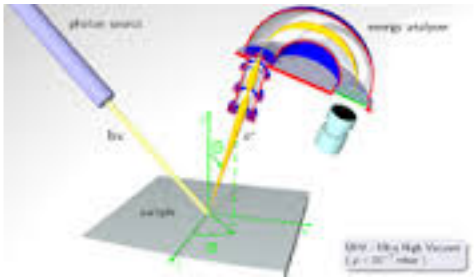
$$K_x = \frac{2mE_{kin}sin\theta cos\phi}{\hbar}$$

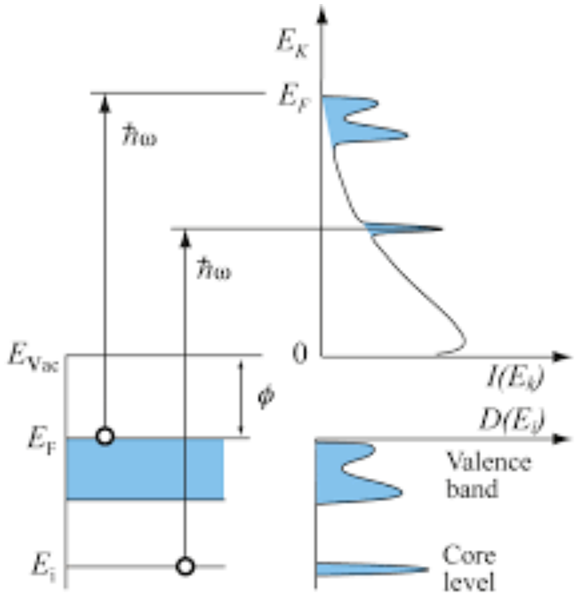
$$K_y = \frac{2mE_{kin}sin\theta sin\phi}{\hbar}$$

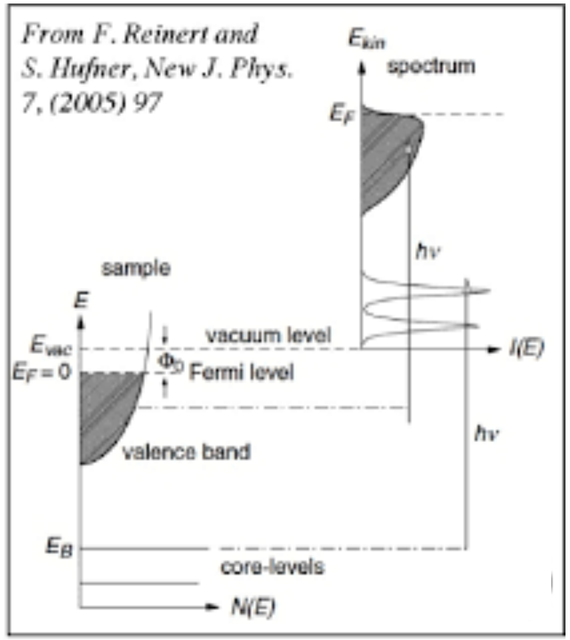
$$K_z = \frac{2mE_{kin}cos\theta}{\hbar}$$

The experiment determines the momentum of photoelectron in vacuum

PES Experiment

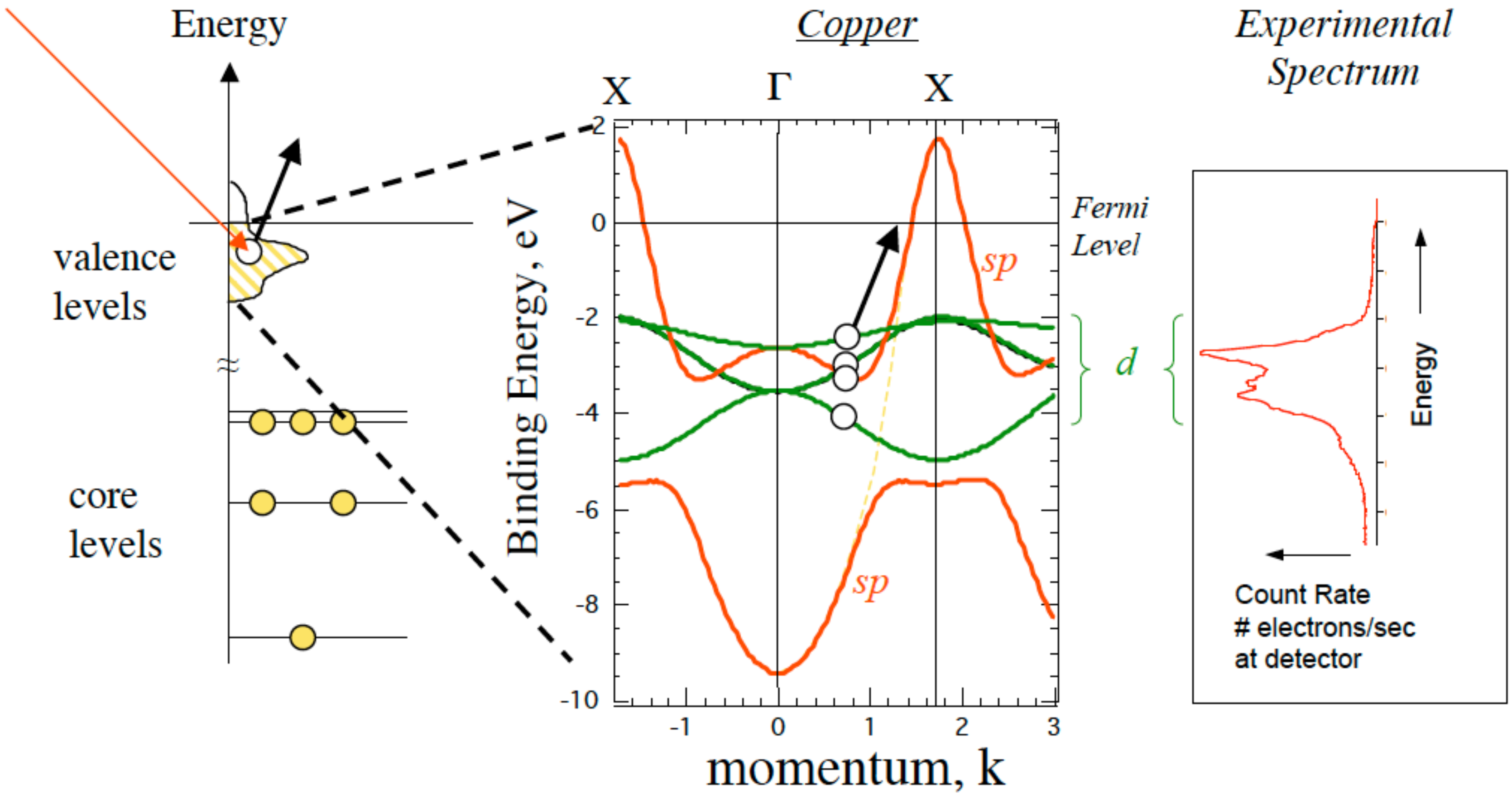




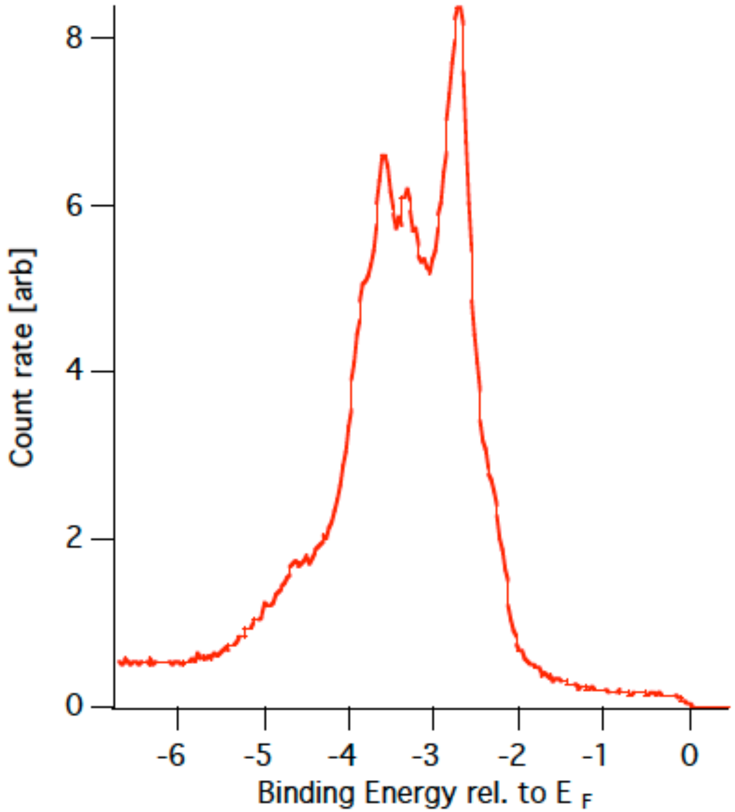


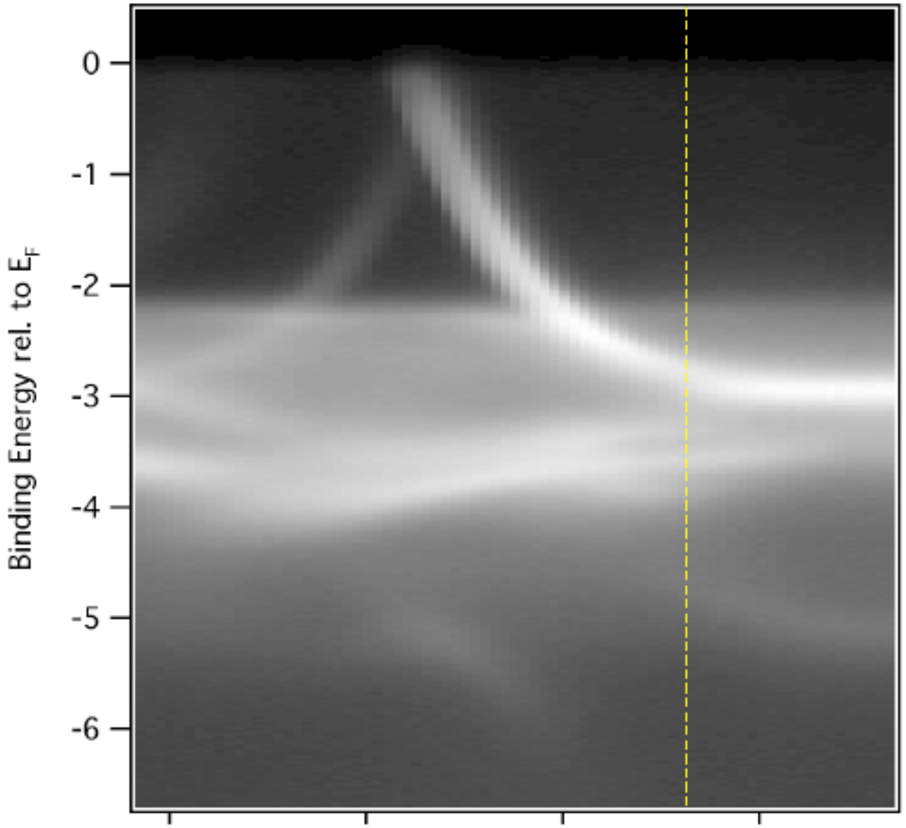
$$h\nu = E_{kin} + E_B + \phi$$

PES Experiment



2D-PES Experiment

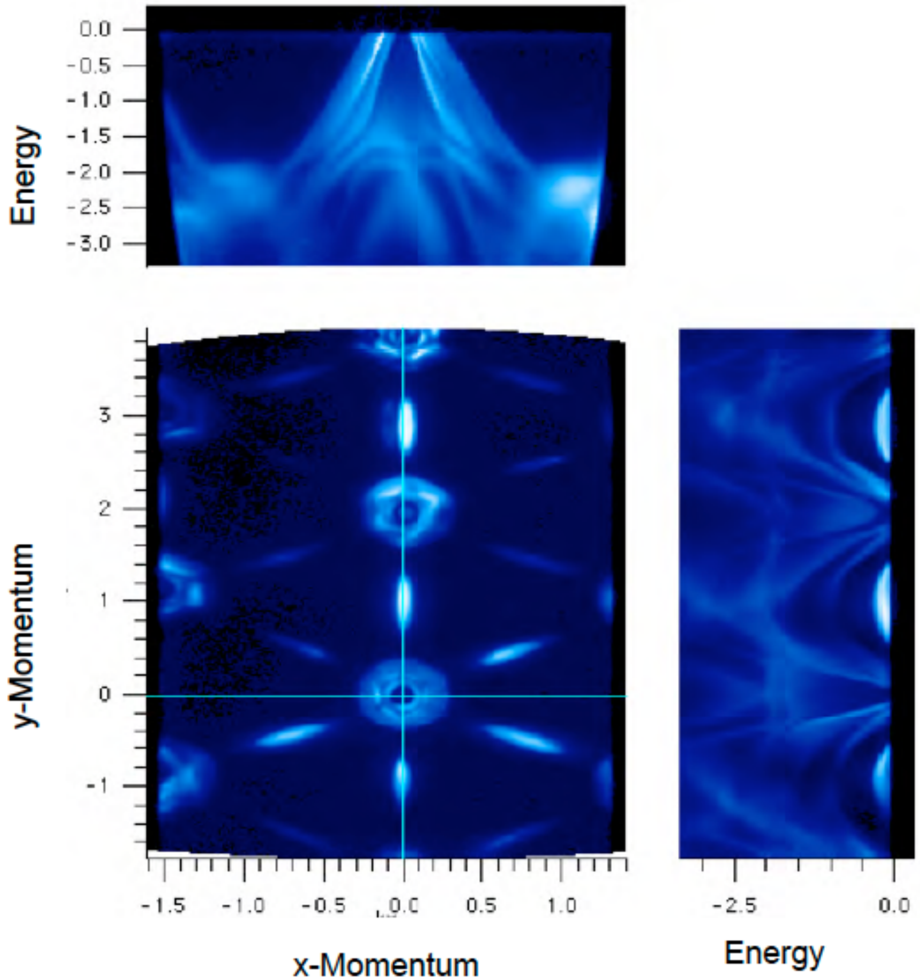




A spectrum at a single momentum k_x

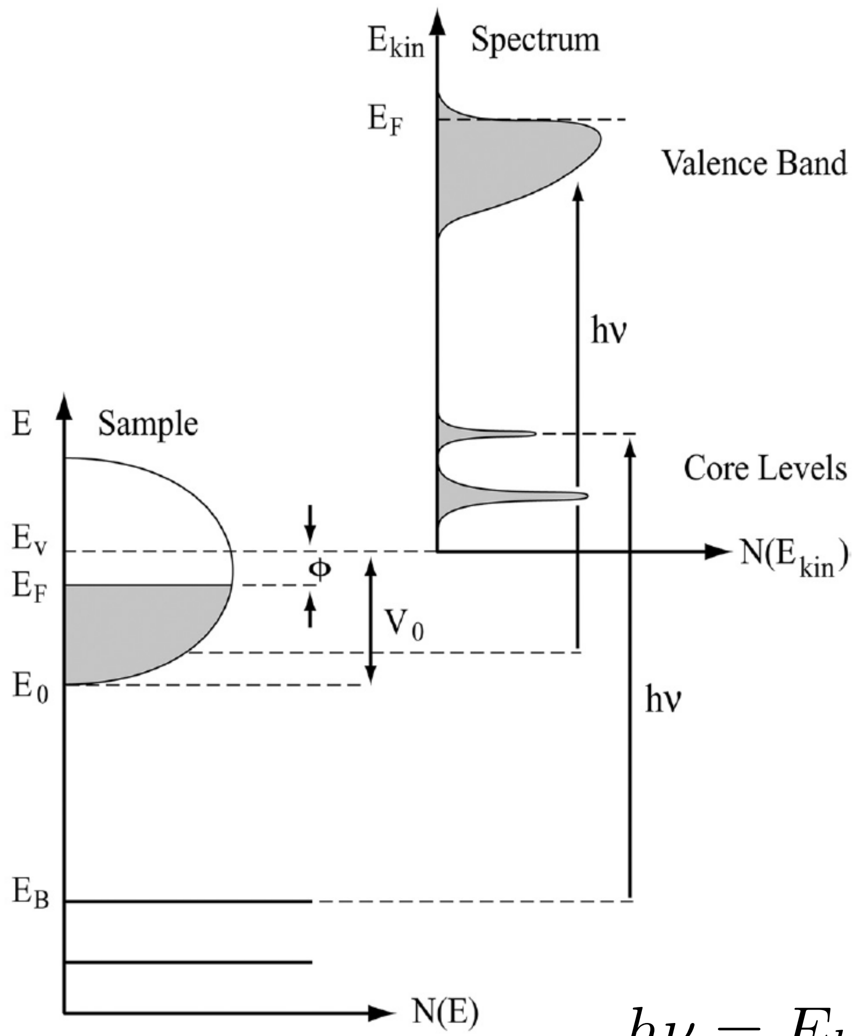
Accumulate spectra as the momentum k_x is scanned

3D-PES Experiment



TiTe2 data courtesy K. Rossnagel, U. Kiel

PES – determining momentum

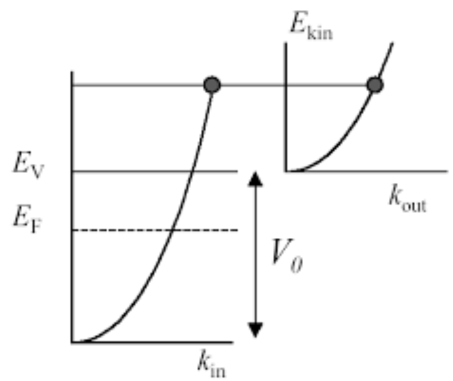


Translation symmetry in *x-y*

$$k_{\|} = K_{\|} = \frac{\sqrt{2mE_{kin}}}{\hbar} sin\theta$$

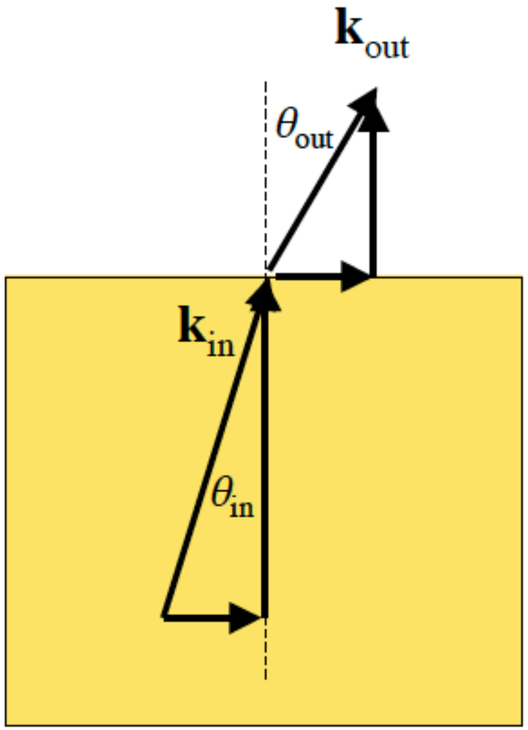
Unknown V_0

$$k_{\perp} = \frac{\sqrt{2m(E_{kin}cos^2\theta + V_0)}}{\hbar}$$



$$h\nu = E_{kin} + E_B + \phi$$

PES – determining momentum



Kinematic relations

$$E_{kinetic} = h\nu - E$$

$$k_{out} = \sqrt{\frac{2m}{\hbar^2} E_{kin}}$$

$$k_{in} = \sqrt{\frac{2m}{\hbar^2}(E_{kin} + V_0)}$$

$$k_{out,\parallel} = k_{in,\parallel} \equiv k_\parallel$$

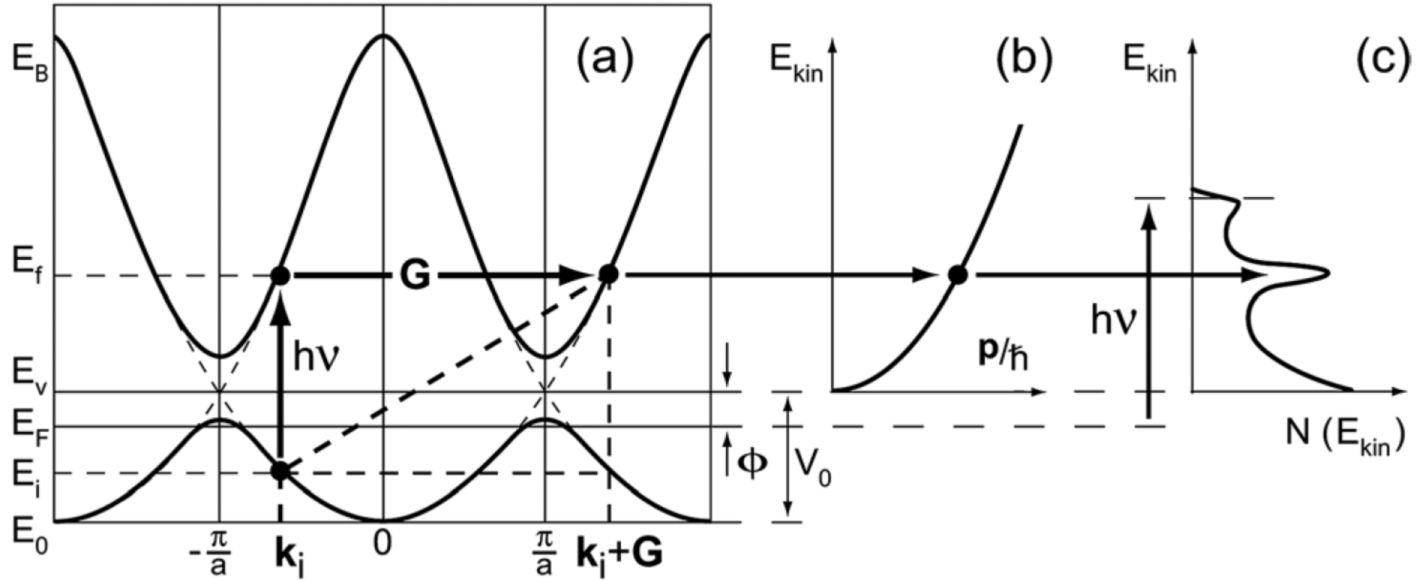
"Snell's Law"

$$k_\parallel = \sin\theta_{out}\sqrt{\frac{2m}{\hbar^2} E_{kin}} = \sin\theta_{in}\sqrt{\frac{2m}{\hbar^2}(E_{kin} + V_0)}$$

Critical angle for emission

$$(\sin\theta_{out})_{\max} = \sqrt{\frac{E_{kin}}{E_{kin} + V_0}}$$

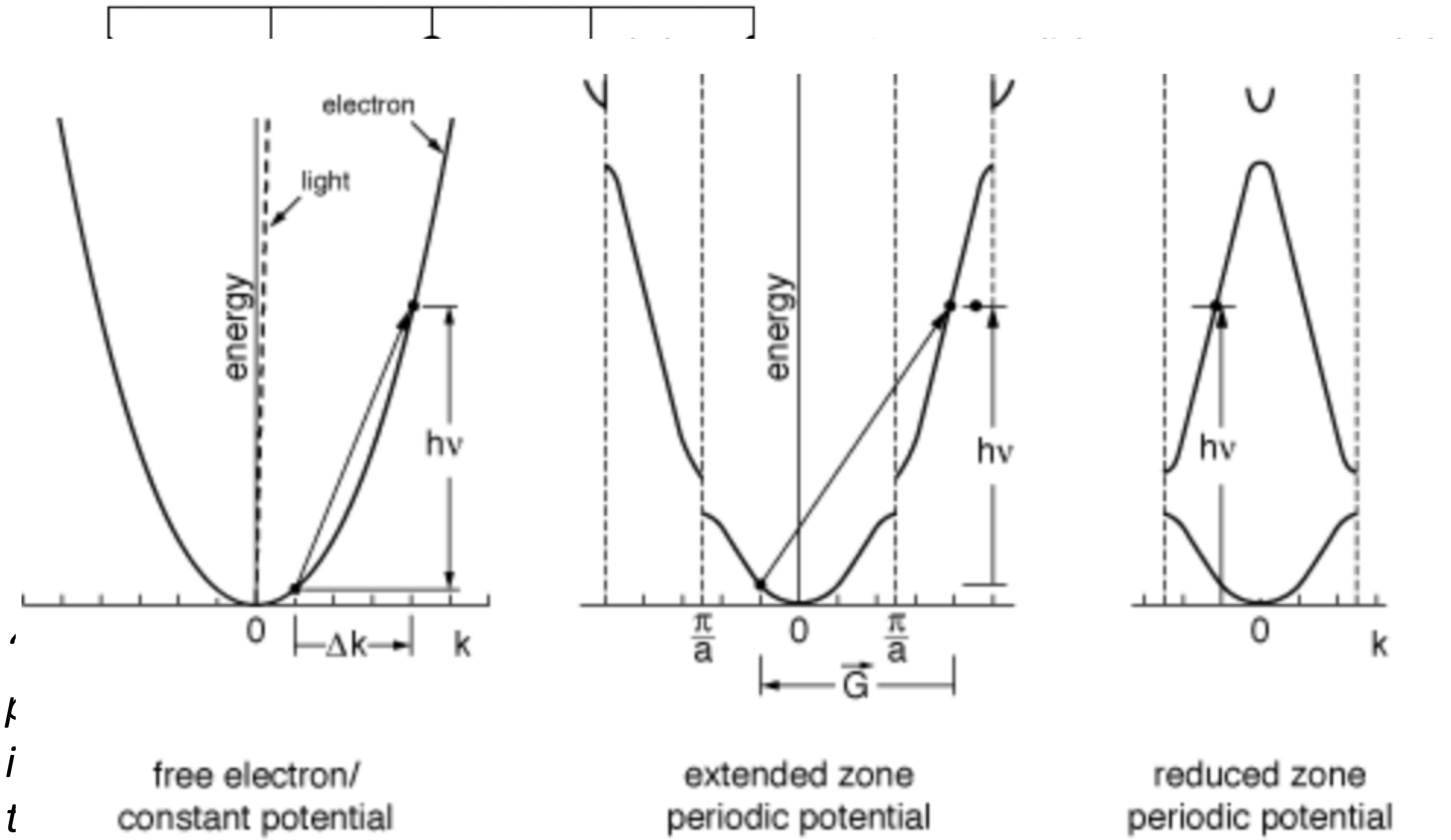
PES – kinematics



*"…in a nearly-free-electron gas, optical absorption may be viewed a two-step process. The absorption of the photon provides the electron with additional energy it needs to get to the excited state. The crystal potential imparts to the electron to the electron the additional momentum it needs to reach the excited state. This momentum comes in the multiples of the reciprocal-lattice vector **G.** So in a reduced zone picture, the transitions are vertical in wave-vector space. **But in photoemission, it is more useful to think in an extended-zone scheme.***

G. D. Mahan, Phys. Rev. B, 1970

PES – kinematics

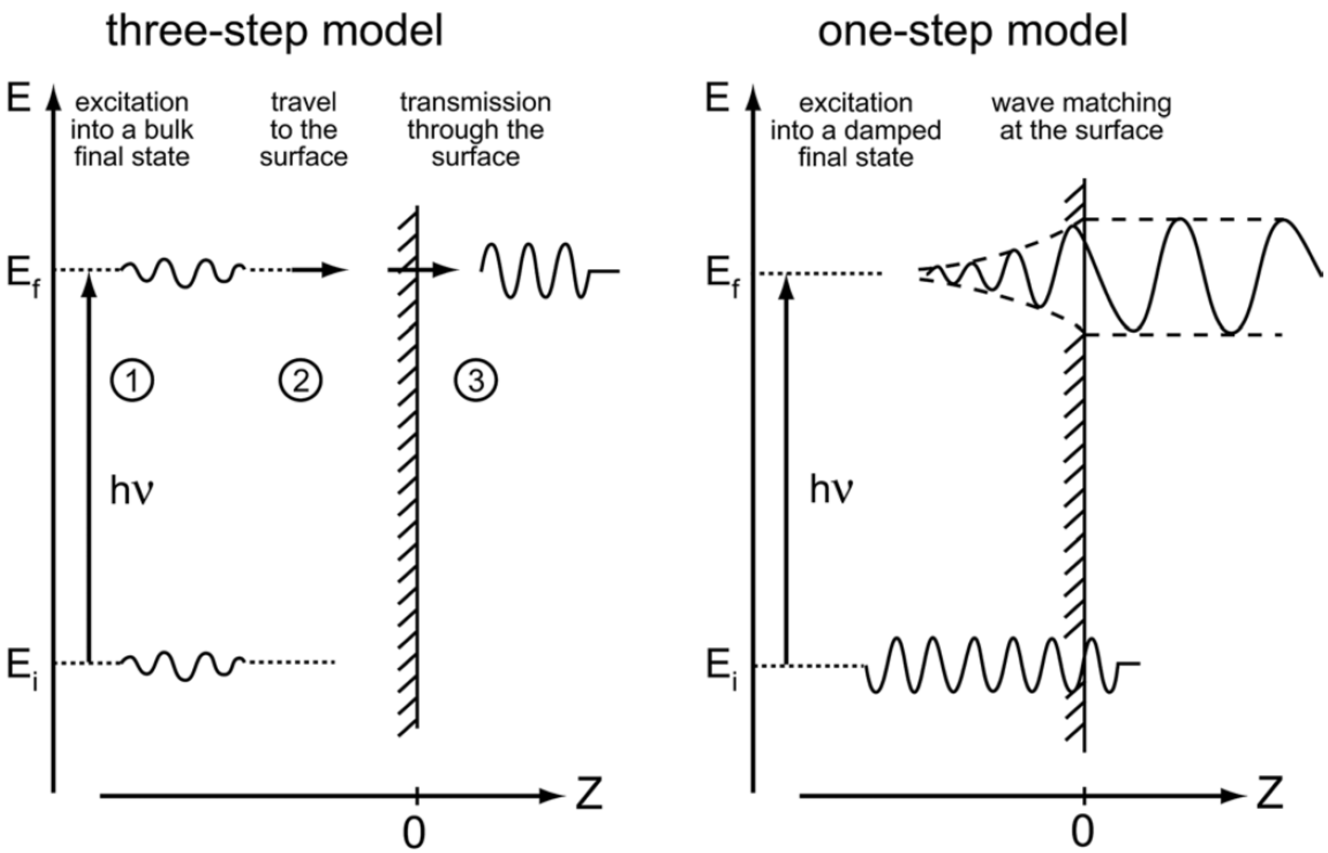


Momentum conservation in angle-resolved photoemission.

it is more useful to think in an extended-zone scheme.

G. D. Mahan, Phys. Rev. B, 1970

Three- and one-step models



Three-Step Model

- 1. Optical excitation

$$\left|\langle \Psi_f^N | H_{int} | \Psi_i^N \rangle\right|^2 \times \delta\left(E_f^N - E_i^N - \hbar\omega\right) \times \left(k_i - G - K\right)$$

$$H_{int} = \frac{e}{2mc}\left(A \cdot p\right)$$

- 2. Travel to the surface. Only elastic scattering is considered. Mean free path is about a few angstroms.

- 3. Escape by a transmission through the surface.

$$\hbar^2 k_\perp^2 / 2m \geqslant E_0 + \phi$$

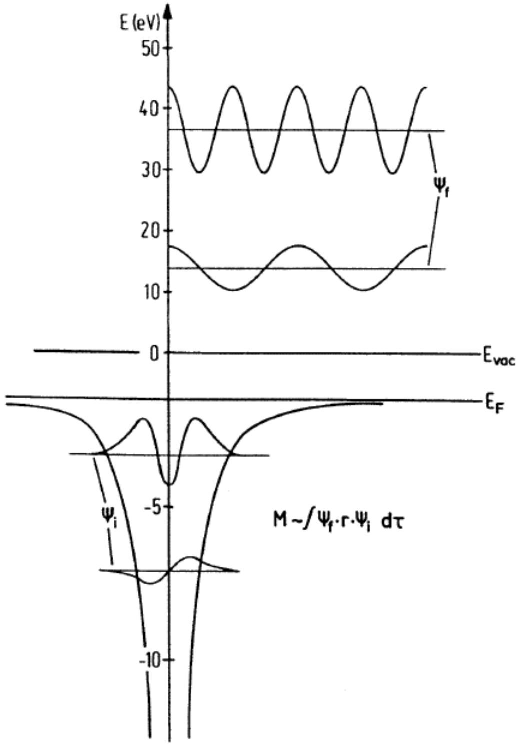
Three-Step Model

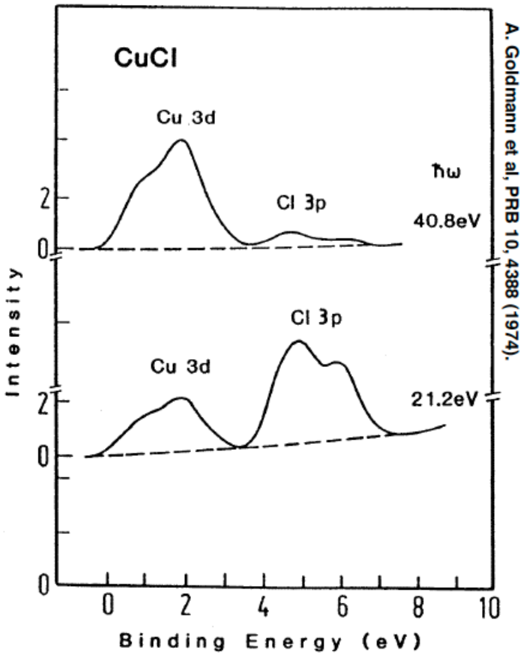
- 1. Optical excitation

$$\left|\langle\Psi_f^N|H_{int}|\Psi_i^N\rangle\right|^2 \times \delta\left(E_f^N - E_i^N - \hbar\omega\right) \times \left(k_i - G - K\right)$$

$$H_{int} = \frac{e}{2mc}\left(A \cdot p\right)$$

- 2. Tra… Mean free path i…





- 3. Esc…

Three-Step Model

- 1. Optical excitation

$$\left|\langle\Psi_f^N|H_{int}|\Psi_i^N\rangle\right|^2 \times \delta\left(E_f^N - E_i^N - \hbar\omega\right) \times \left(k_i - G - K\right)$$

$$H_{int} = \frac{e}{2mc}\left(A \cdot p\right)$$

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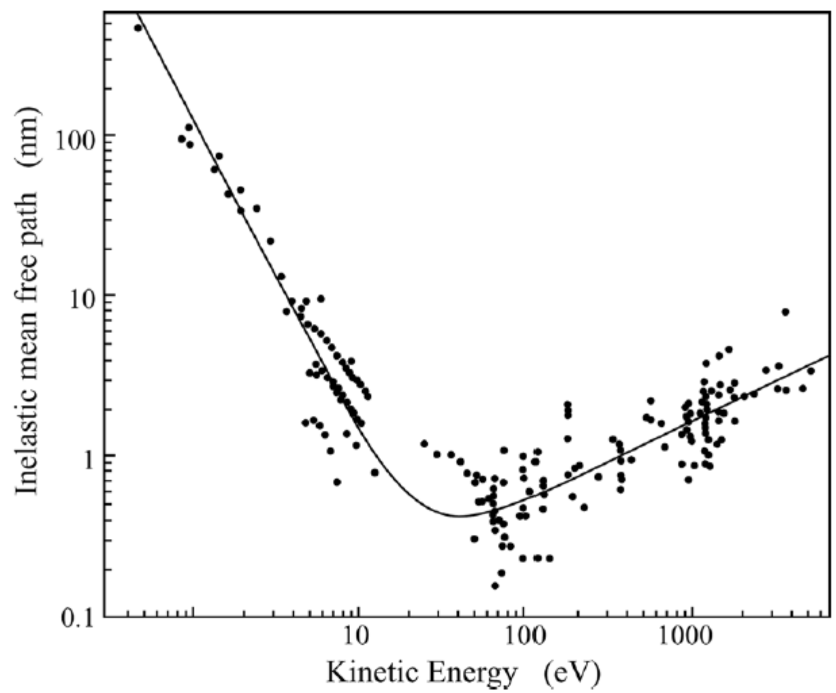
Three



- 1. Optical excitation

$$\left|\langle\Psi_f^N|H_{int}|\Psi_i^N\rangle\right|^2 \times \delta\left(E_f^N - E\right.$$

$$H_{int} = \frac{e}{2m}$$

- 2. Travel to the surface. Only elastic scattering is considered. Mean free path is about a few angstroms.

- 3. Escape by a transmission through the surface.

$$\hbar^2 k_\perp^2/2m \geqslant E_0 + \phi$$

Three-Step Model

- 1. Optical excitation

$$\left|\langle\Psi_f^N|H_{int}|\Psi_i^N\rangle\right|^2 \times \delta\left(E_f^N - E_i^N - \hbar\omega\right) \times \left(k_i - G - K\right)$$

$$H_{int} = \frac{e}{2mc}\left(A \cdot p\right)$$

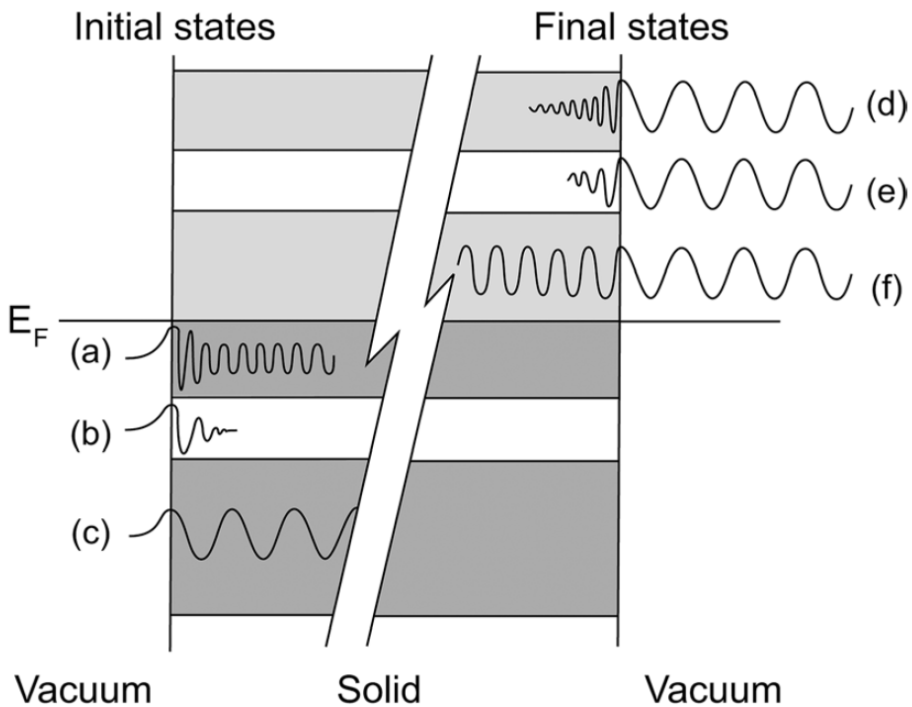
- 2. Travel to the surface. Only elastic scattering is considered. Mean free path is about a few angstroms.

- 3. Escape by a transmission through the surface.

$$\hbar^2 k_\perp^2/2m \geqslant E_0 + \phi$$

One-Step Model

Electron excitation, removal and detection a single *coherent* process



One-Step Model

$$H_{int} = \frac{e}{2mc}\left(\mathbf{A}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{A}\right) = \frac{e}{2mc}\left(\mathbf{A}\cdot\mathbf{p}\right)$$

linear optical regime, dipole approximation

Under assumption $\nabla \cdot \mathbf{A} = 0$

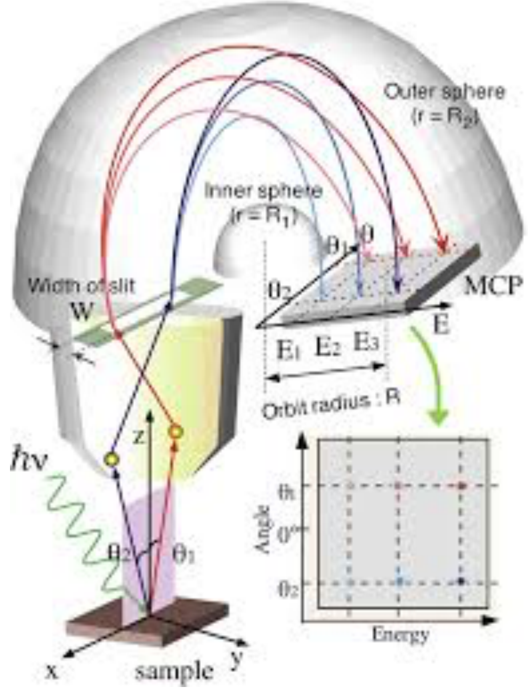
Commutation relation $\left[H_0, \mathbf{p}\right] = i\hbar\nabla V$ where $H_0 = \mathbf{p}^2/2m + V$

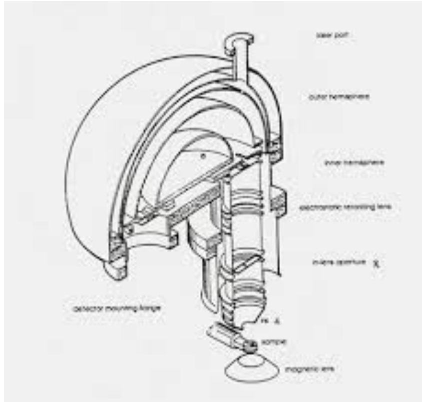
Transition probability $\left\langle \Psi_f^N \middle| \mathbf{A}\cdot\nabla V \middle| \Psi_i^N \right\rangle$

however, inside the material $\nabla V = 0$

on the surface $\partial V/\partial z \neq 0$ - *Surface photoelectric effect*

The Experiment - ARPES





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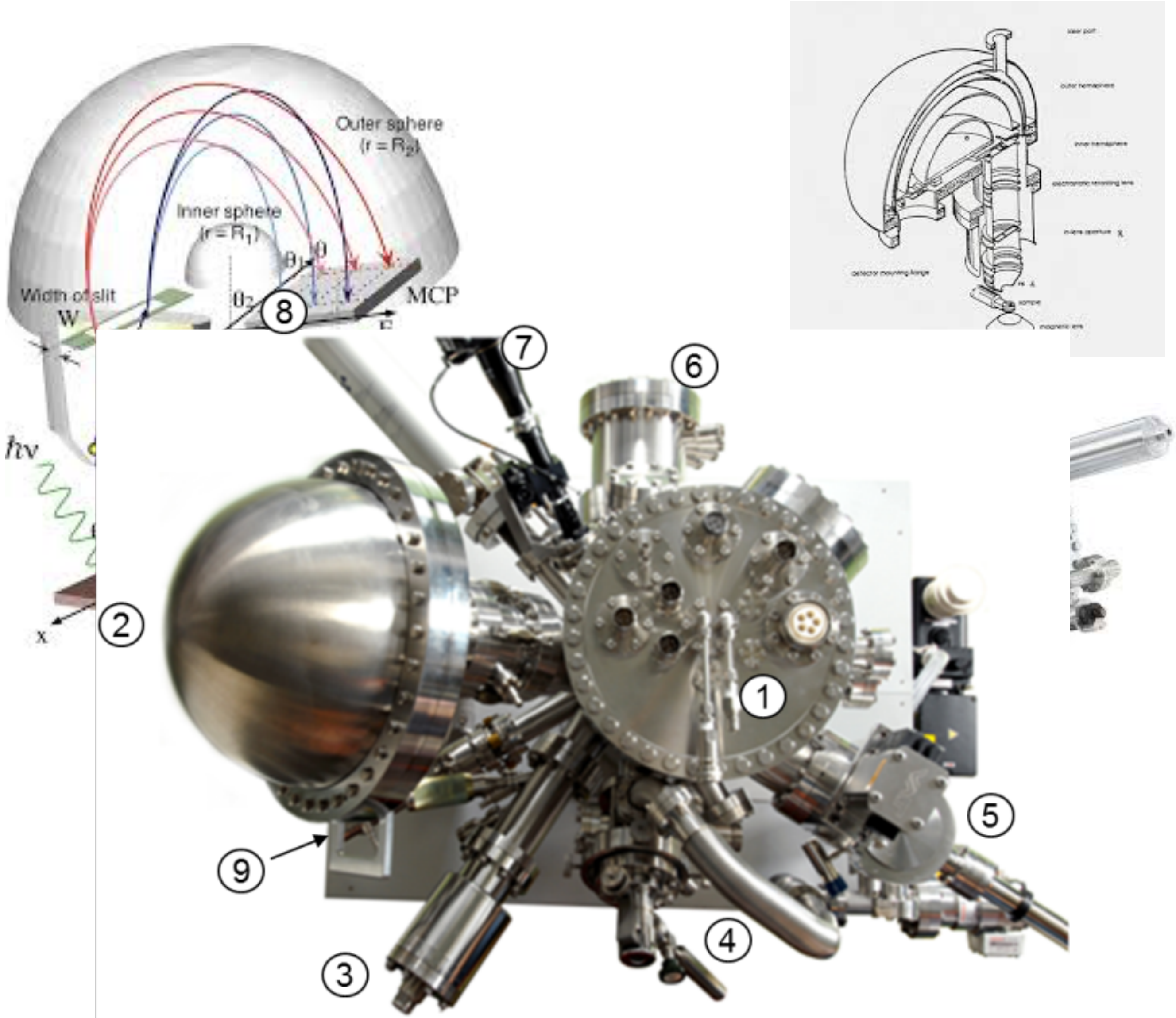
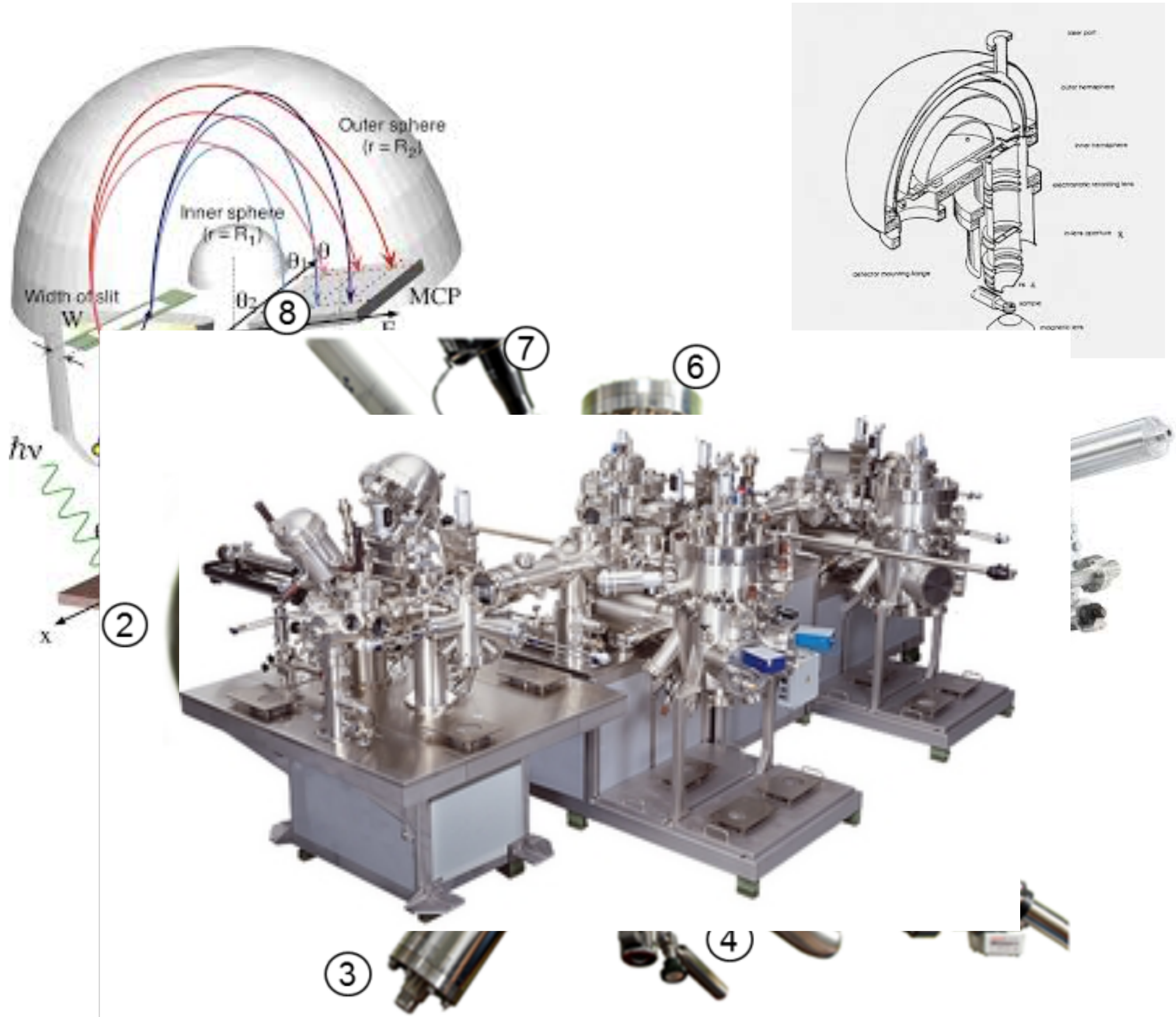
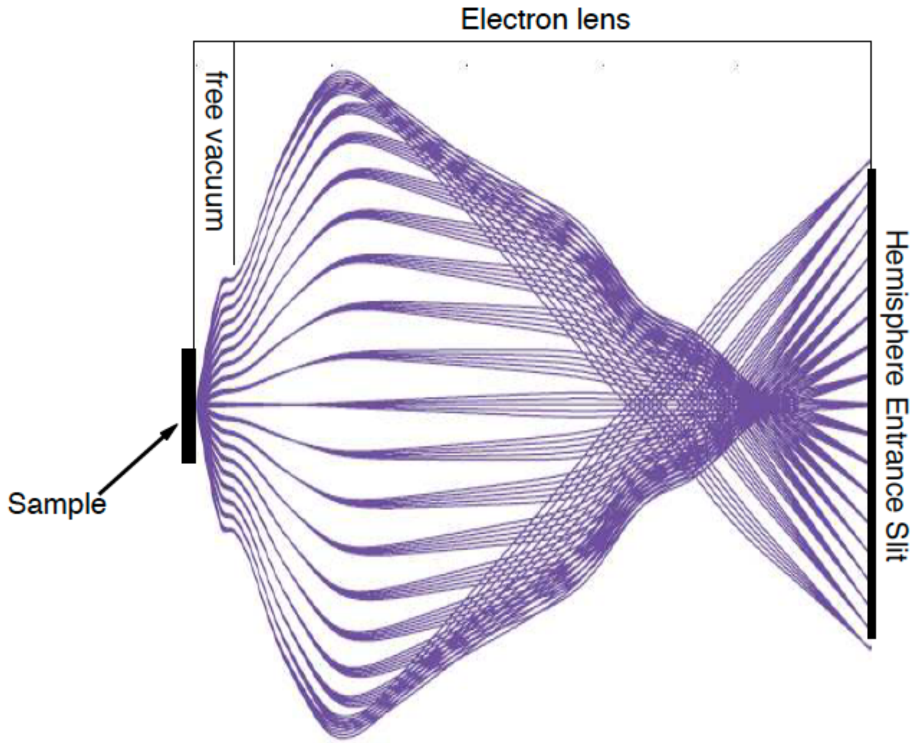


The Experiment - ARPES

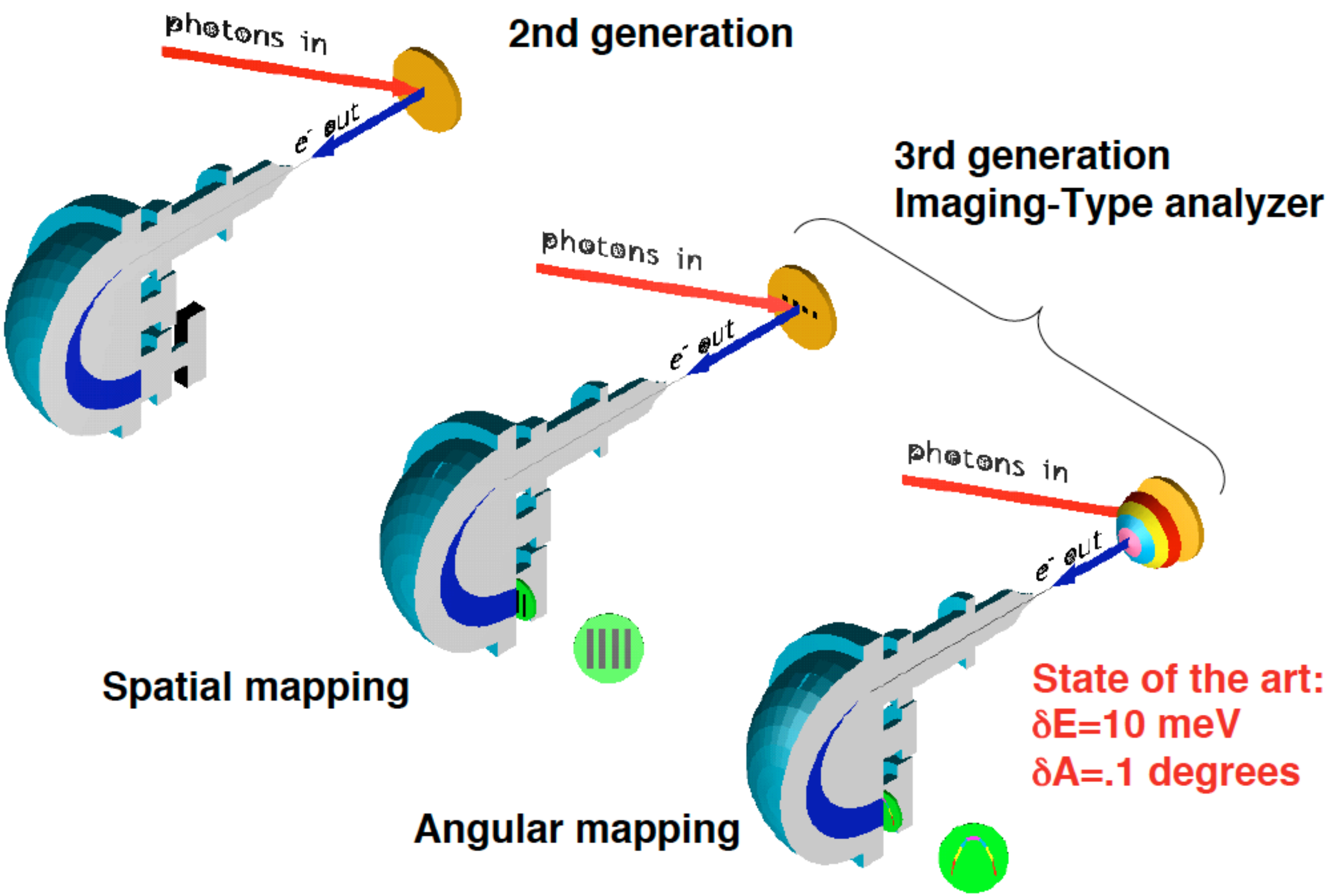


The Experiment - ARPES

Lens



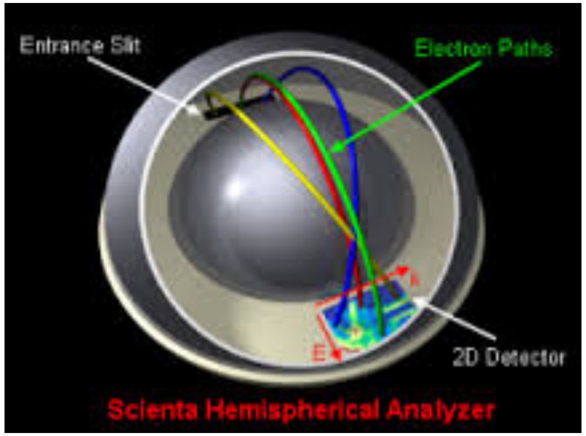
PES-Imaging

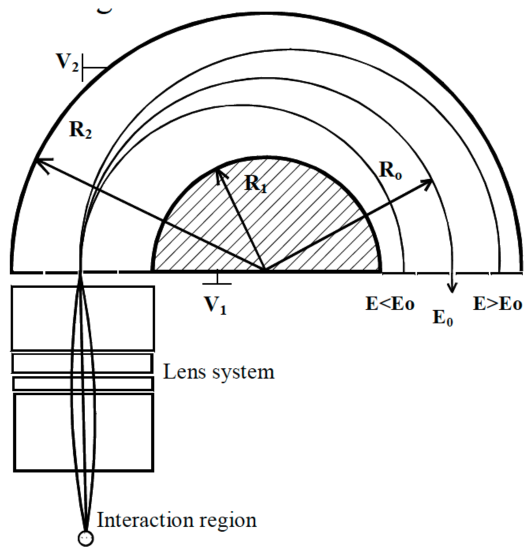


photons in
e⁻ out
2nd generation
3rd generation
Imaging-Type analyzer
photons in
e⁻ out
photons in
e⁻ out
Spatial mapping
Angular mapping
State of the art:
δE=10 meV
δA=.1 degrees

The Experiment - ARPES

Energy Analyzer



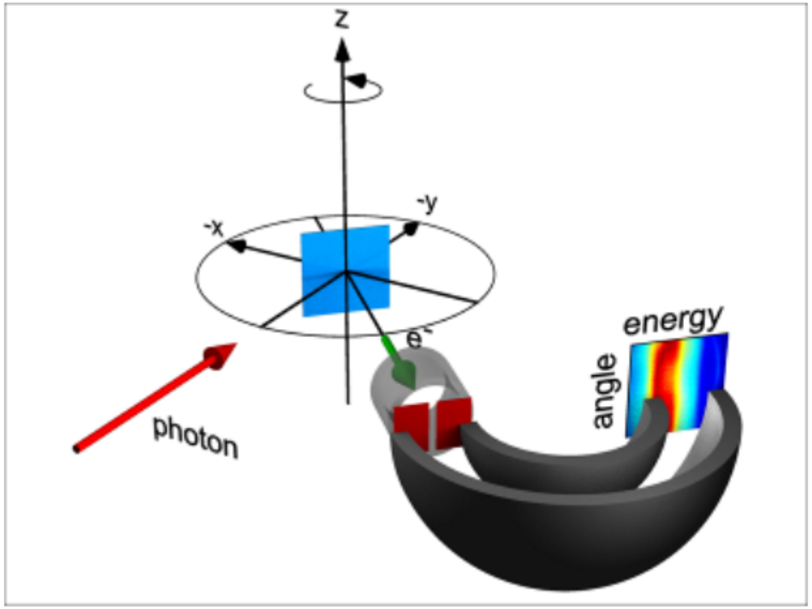


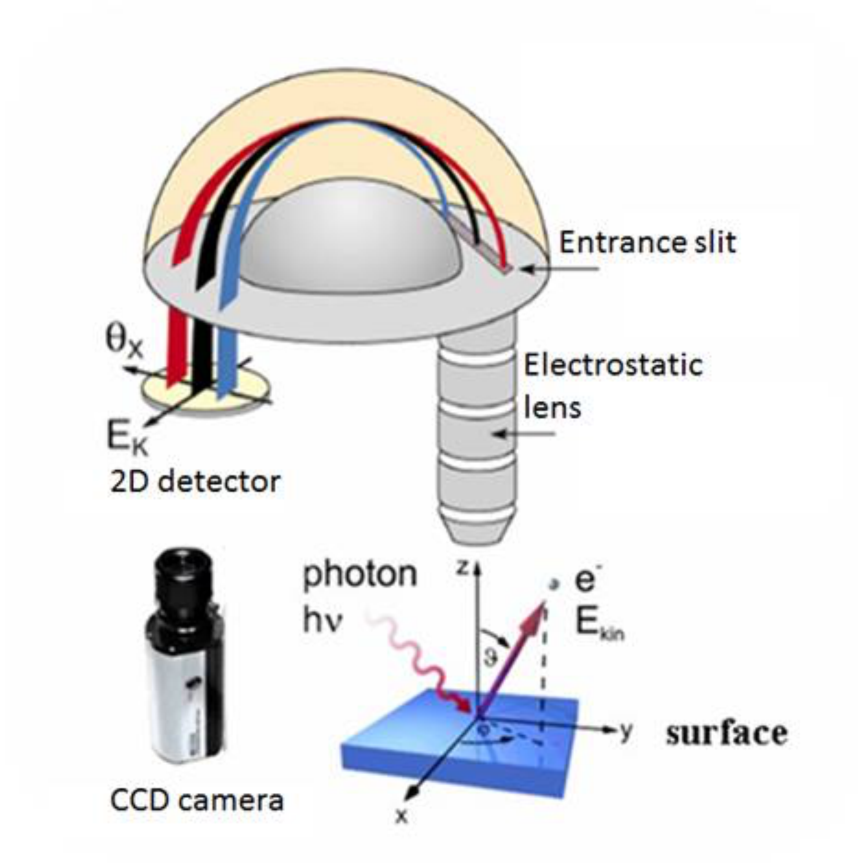
$$V_1(R_1) = V_0\left[\frac{2R_0}{R_1} - 1\right]$$

$$V_2(R_2) = V_0\left[\frac{2R_0}{R_2} - 1\right]$$

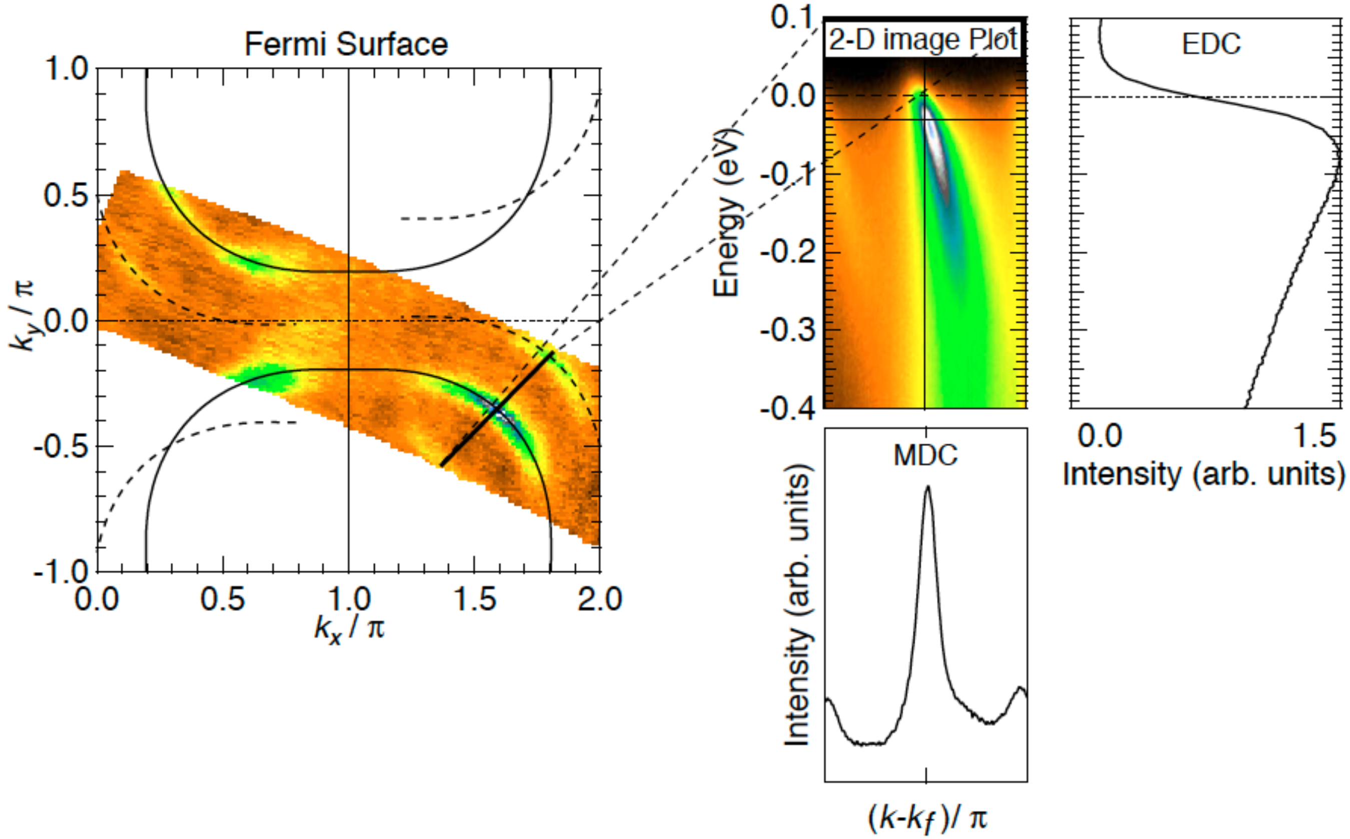
eV_0 - pass energy

The Experiment - ARPES

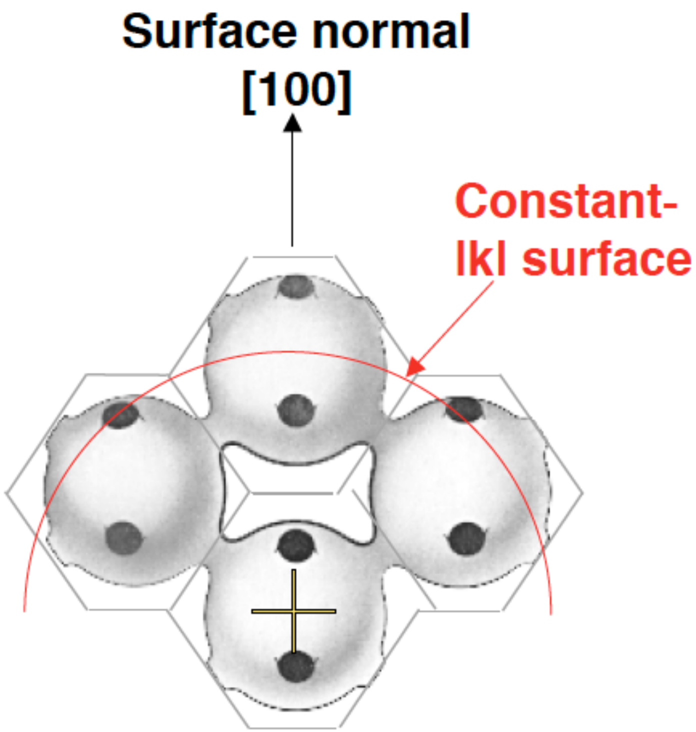




The Experiment - ARPES



ARPES – Cu (100)



$$E_{kinetic} = h\nu = \frac{\hbar^2 k_{out}^2}{2m}$$

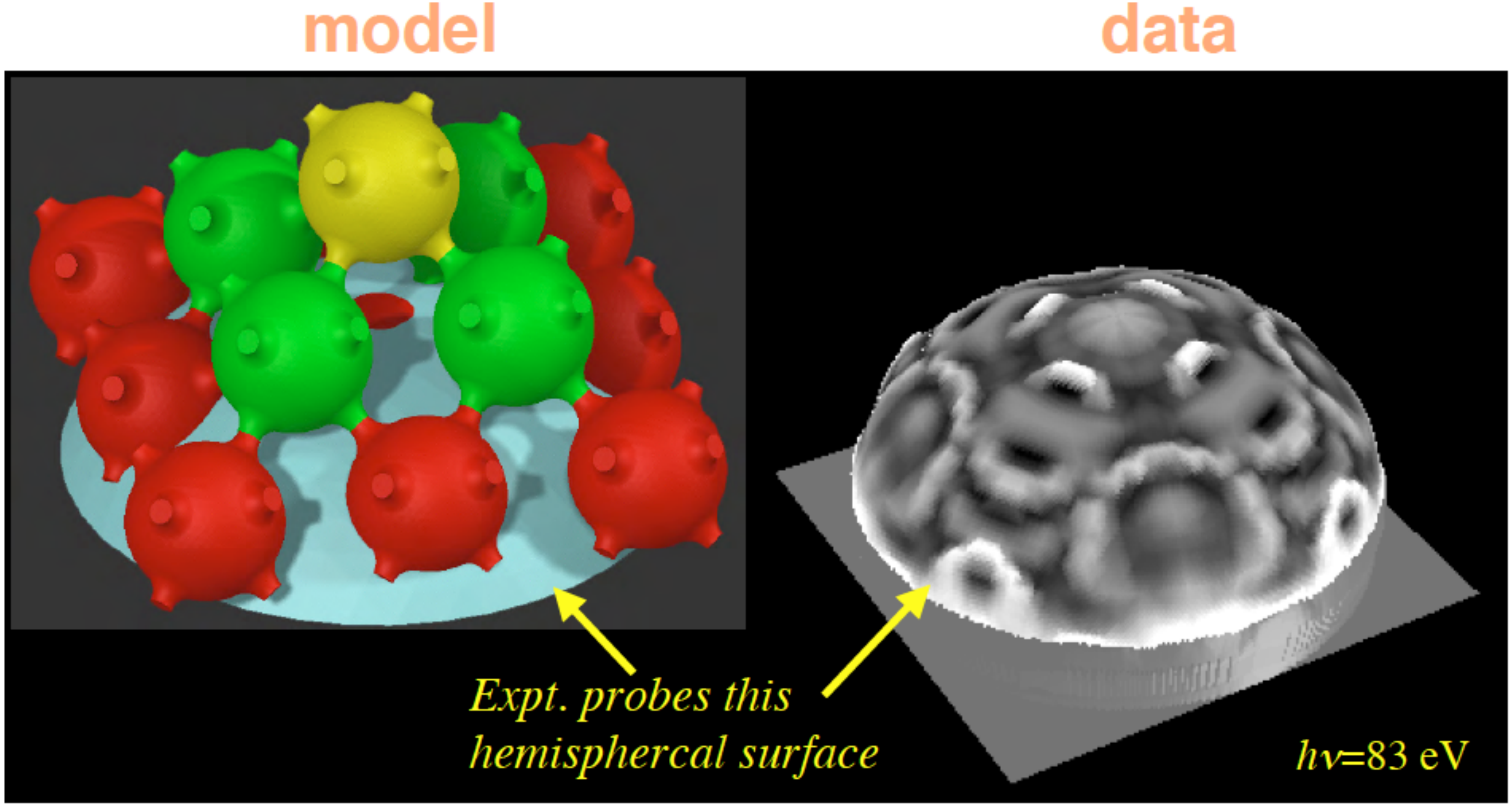
$$k_{out} = \sqrt{\frac{2m}{\hbar^2} E_{kin}}$$

$$k_{in} = \sqrt{\frac{2m}{\hbar^2}(E_{kin} + V_0)}$$

- Fix the photon energy to a constant value, e.g. hν=83 eV and look at the electrons at the Fermi level (zero binding energy)

- The electrons detected have constant $|k_{in}|$ and therefore lie on a sphere in k-space

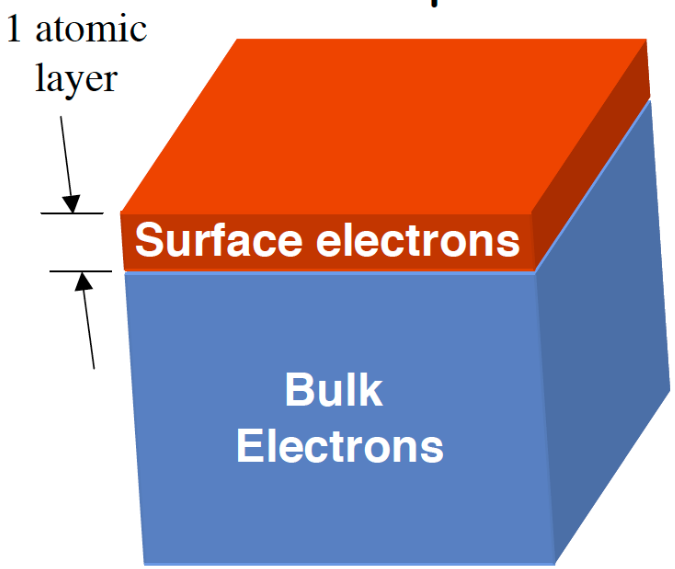
ARPES – Cu (100)



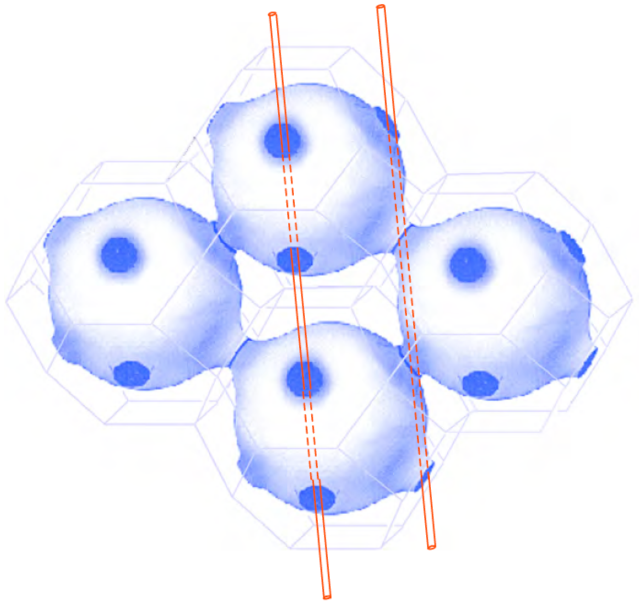
Eli Rotenberg, ALS/LBNL

Surface states

Real Space



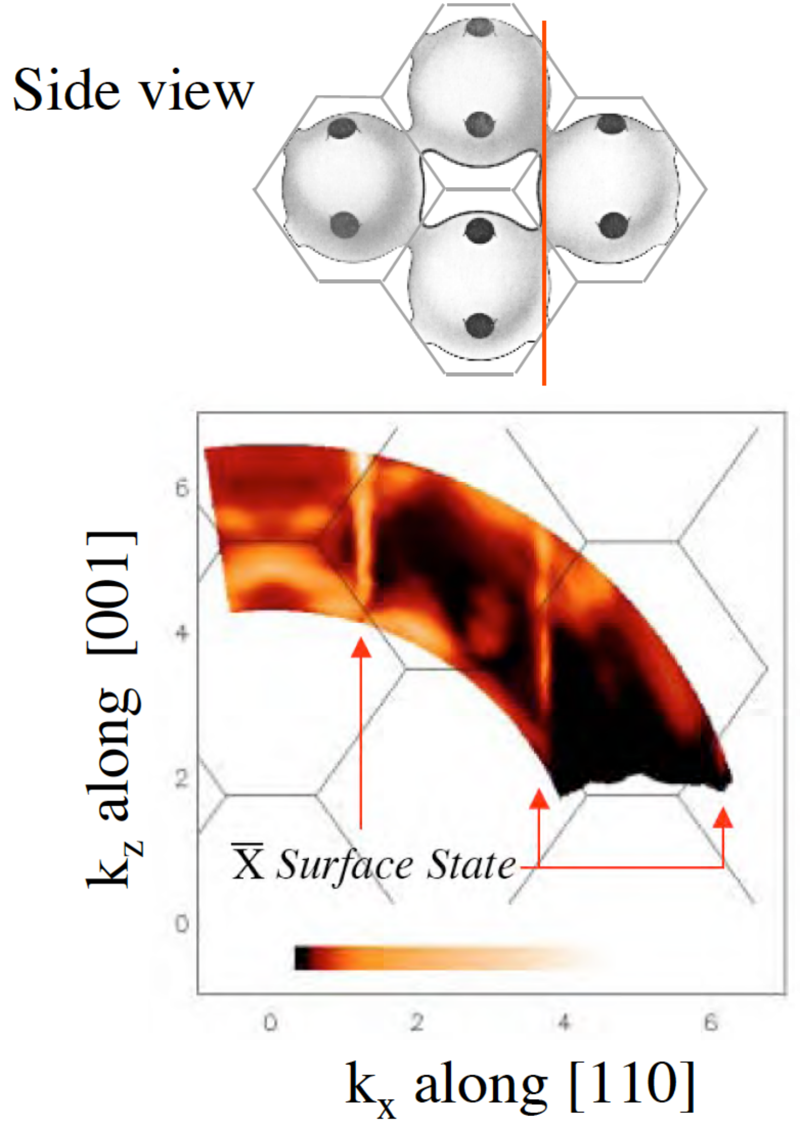
Momentum Space



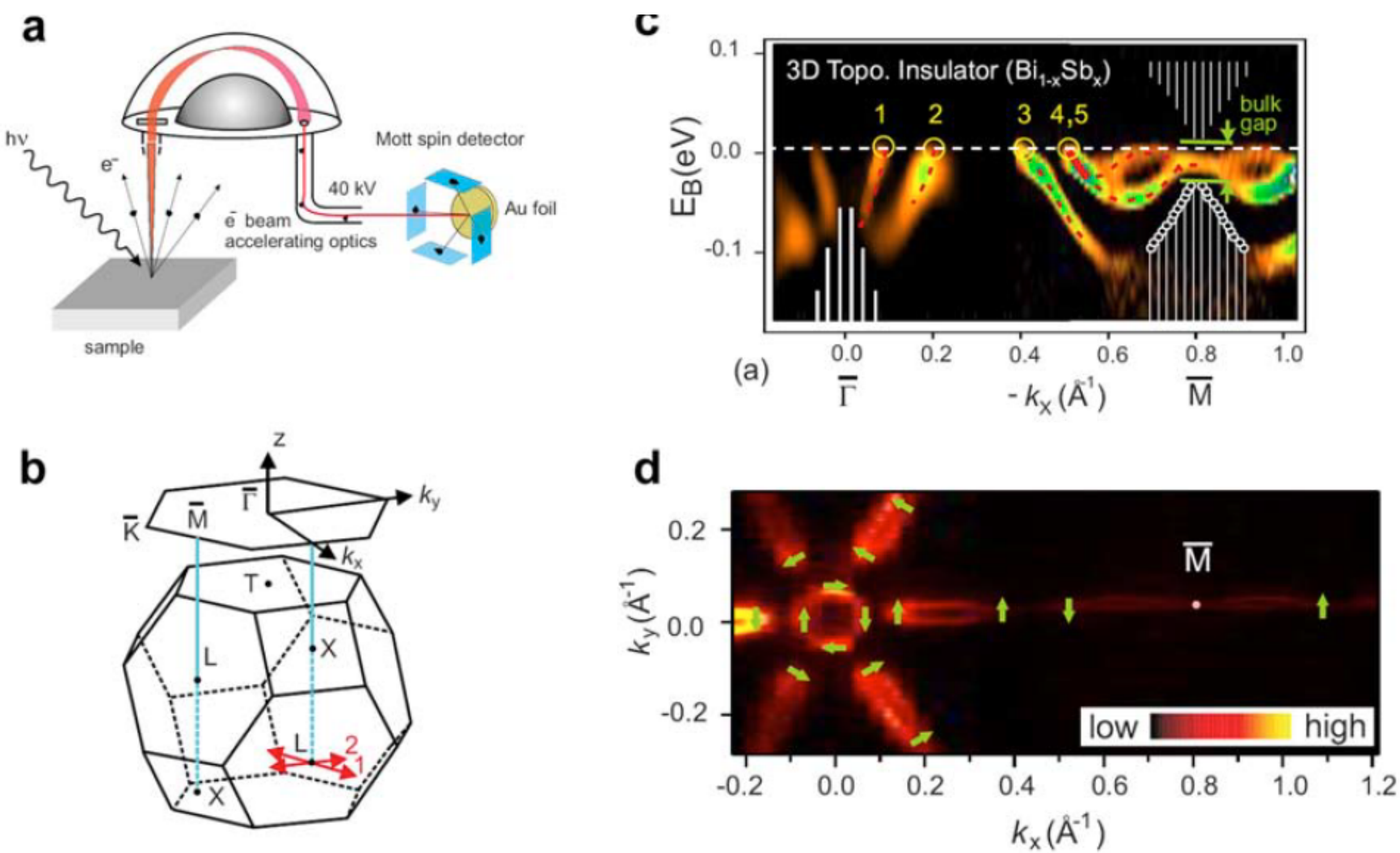
- Surface states are highly localized in real space, therefore completely delocalized in k-space along k_z.
  - NO DISPERSION OF SURFACE STATES in k_z direction

- Energy and momenta of surface and bulk states cannot overlap (otherwise, why would the states be localized to the surface?)

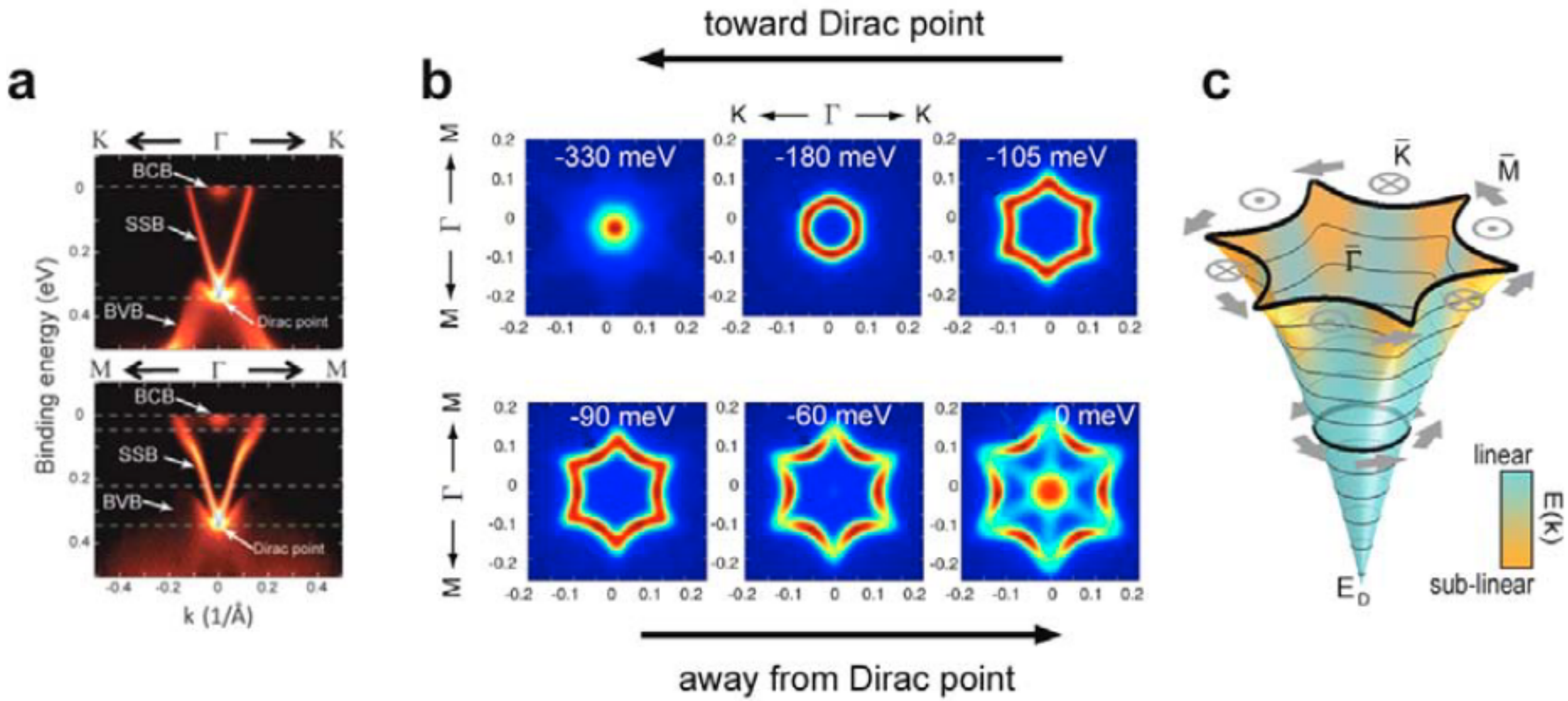
Surface states



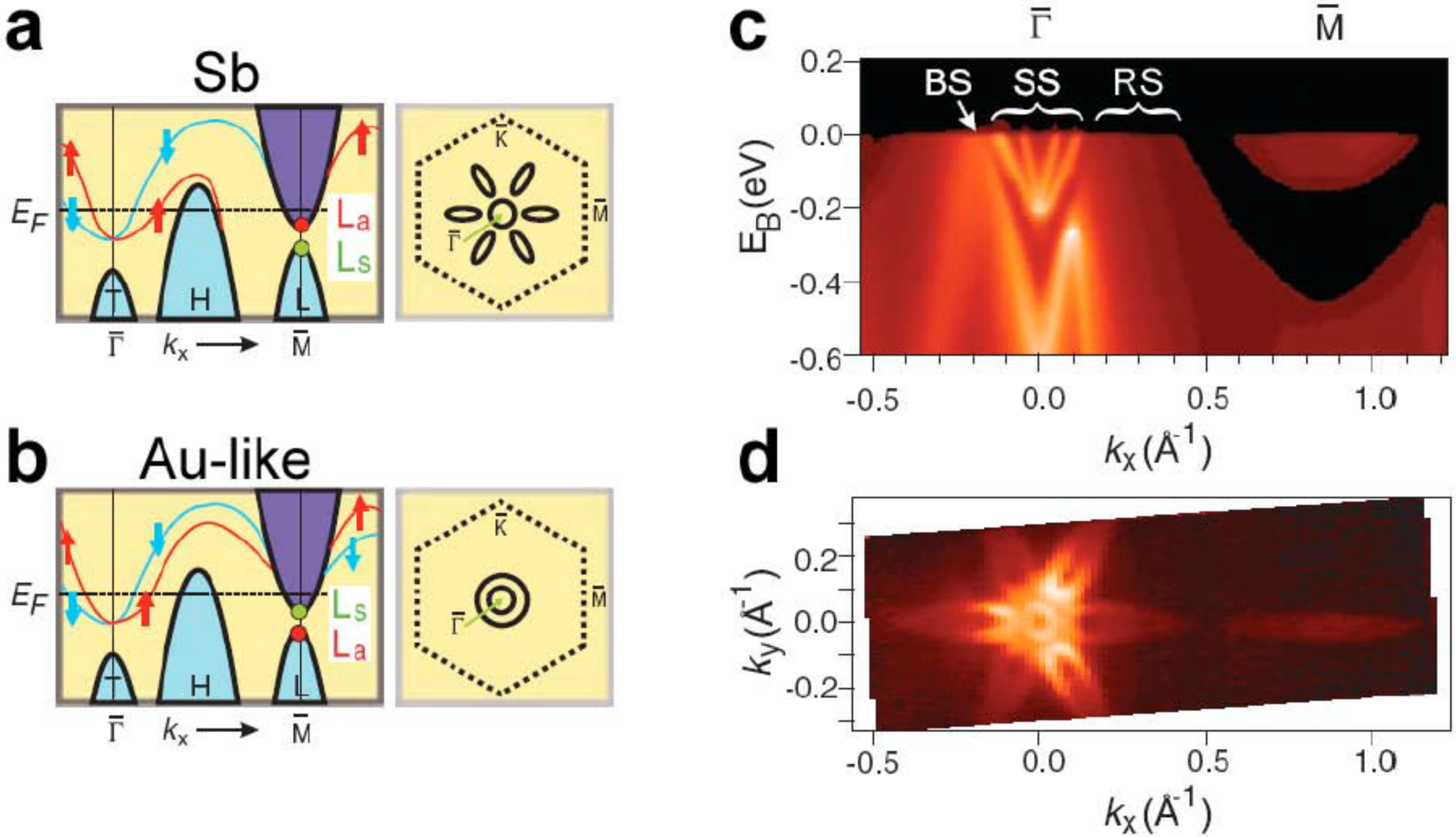
The Experiment - ARPES



Hsieh et al, 2008



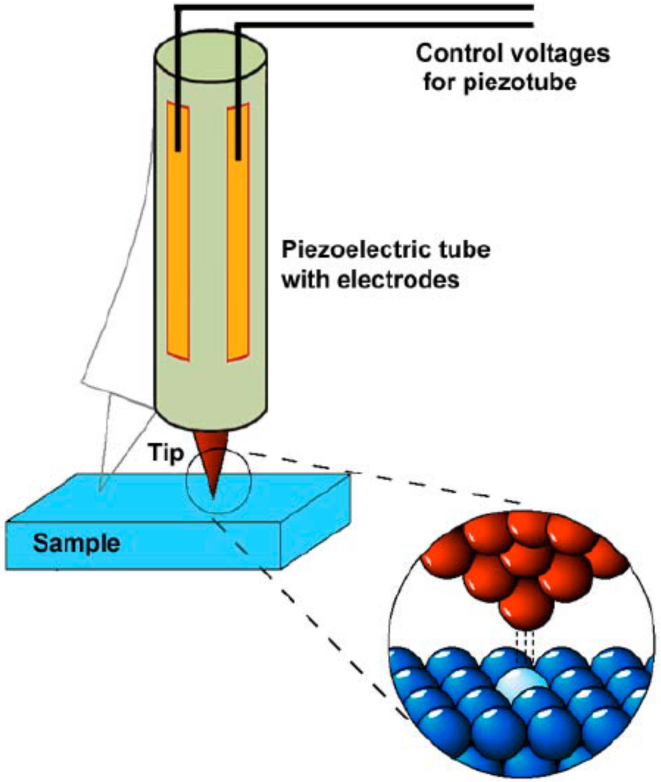
Chen *et al,* Science 2009

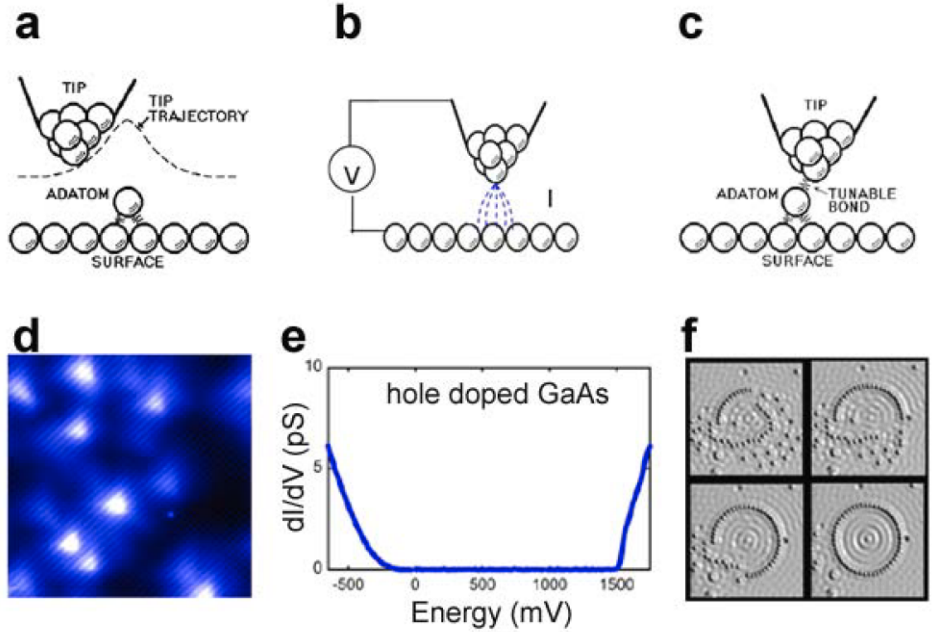


Sb(111)

Hsieh *et al*, Science, 2009

Scanning Tunneling Microscopy





topography LDOS Manipulation

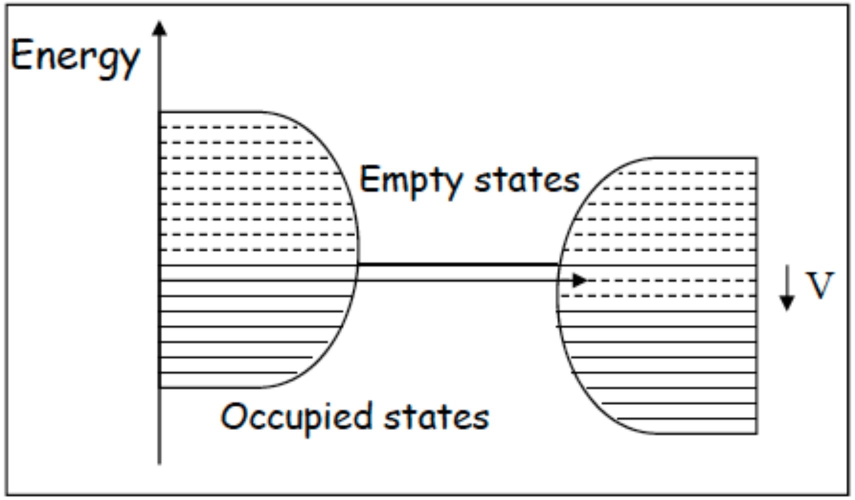
Tunneling Current

Barden, PRL, 1961

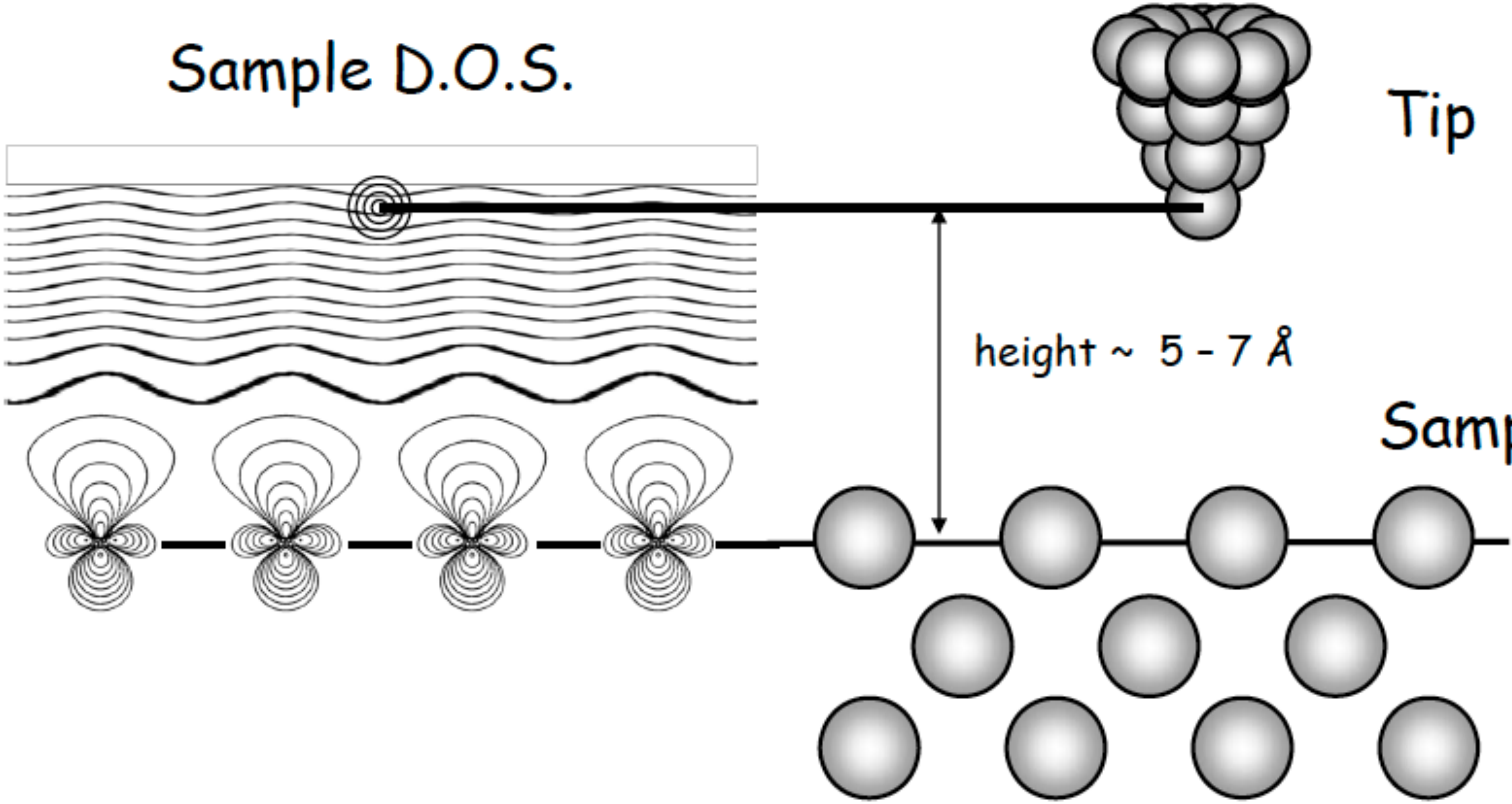
Current (1st order perturbation theory)

$$I_{(k \to k')} = 2\pi e / \hbar \sum_{k,occ.}^{k',empt.} \left|T_{kk'}\right|^2 \delta\left(\varepsilon_k - \varepsilon_{k'}\right)$$

($T_{kk'}$≡tunnelling matrix element between φ_k and $\varphi_{k'}$)

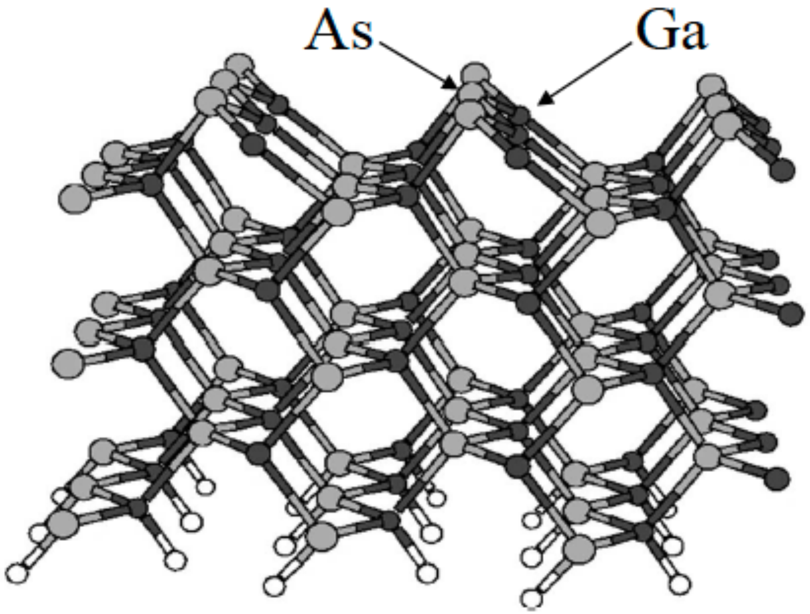


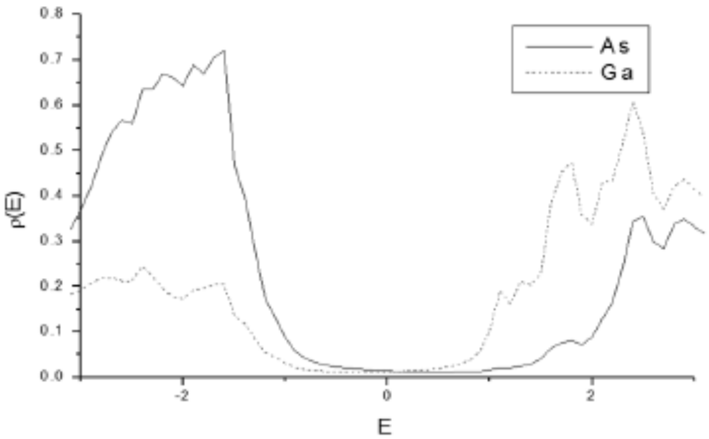
Bardeen showed that under certain assumptions, $T_{kk'} = \hbar/2m \int_S d\vec{S}\,(\varphi_{k'}\vec{\nabla}\,\varphi_k - \varphi_k\vec{\nabla}\,\varphi_{k'})$

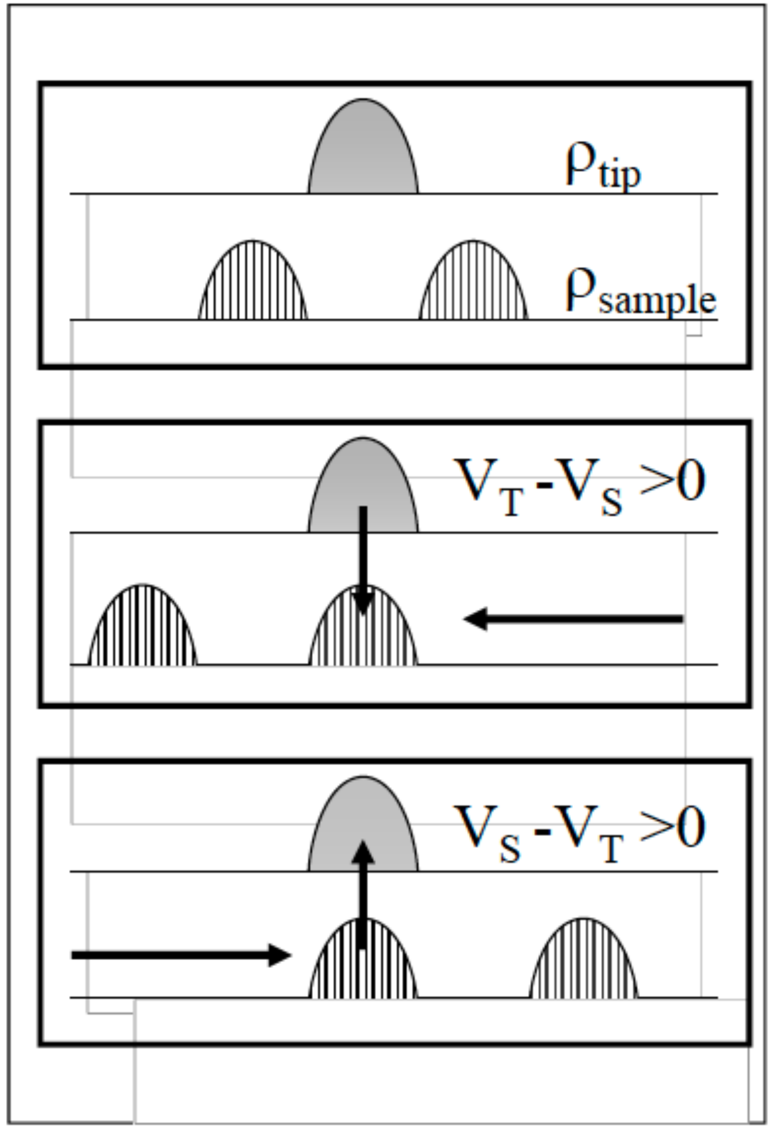


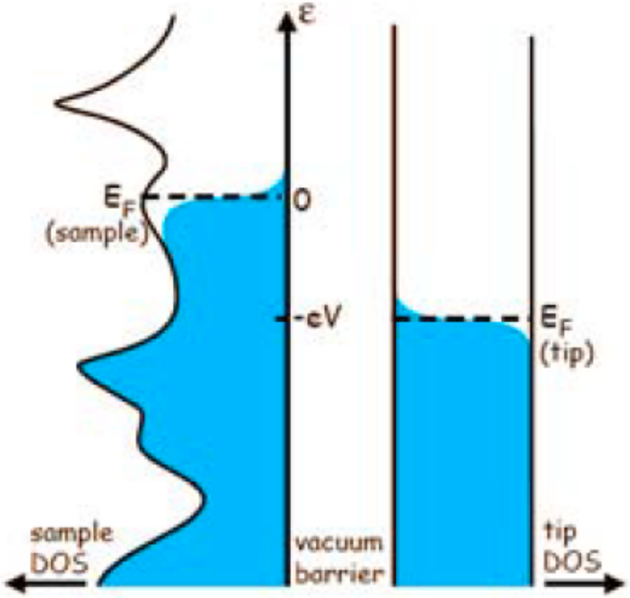
- D.O.S. near the Fermi level controls the current
- STM images are not topographic.

GaAs (110): Understanding the bias dependece





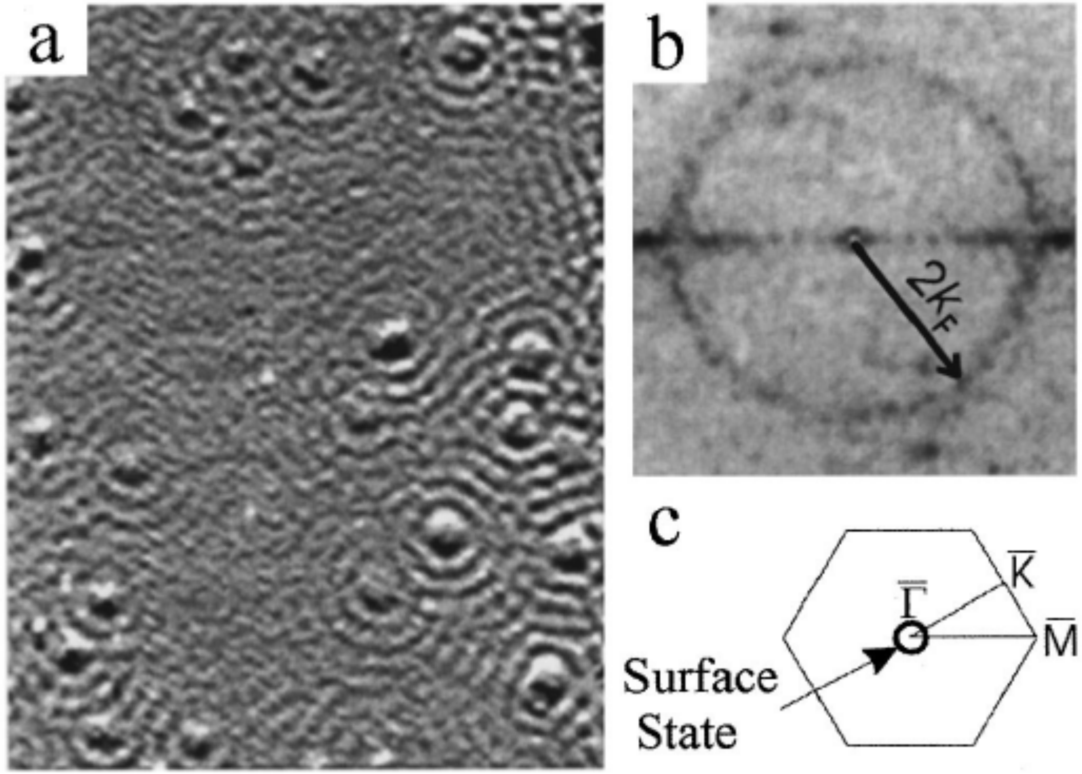




$$I \propto \left|M\right|^2 \rho_T \int_0^{eV} \rho_S(E)dE$$

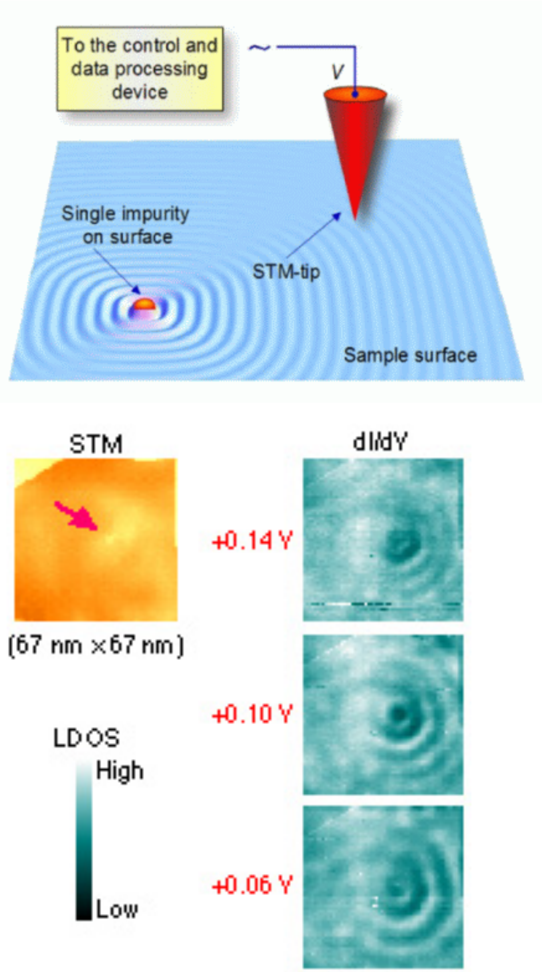
To determine LDOS, measure $$\frac{dI}{dV}$$

Retrieve k-space from STM



Cu(111)

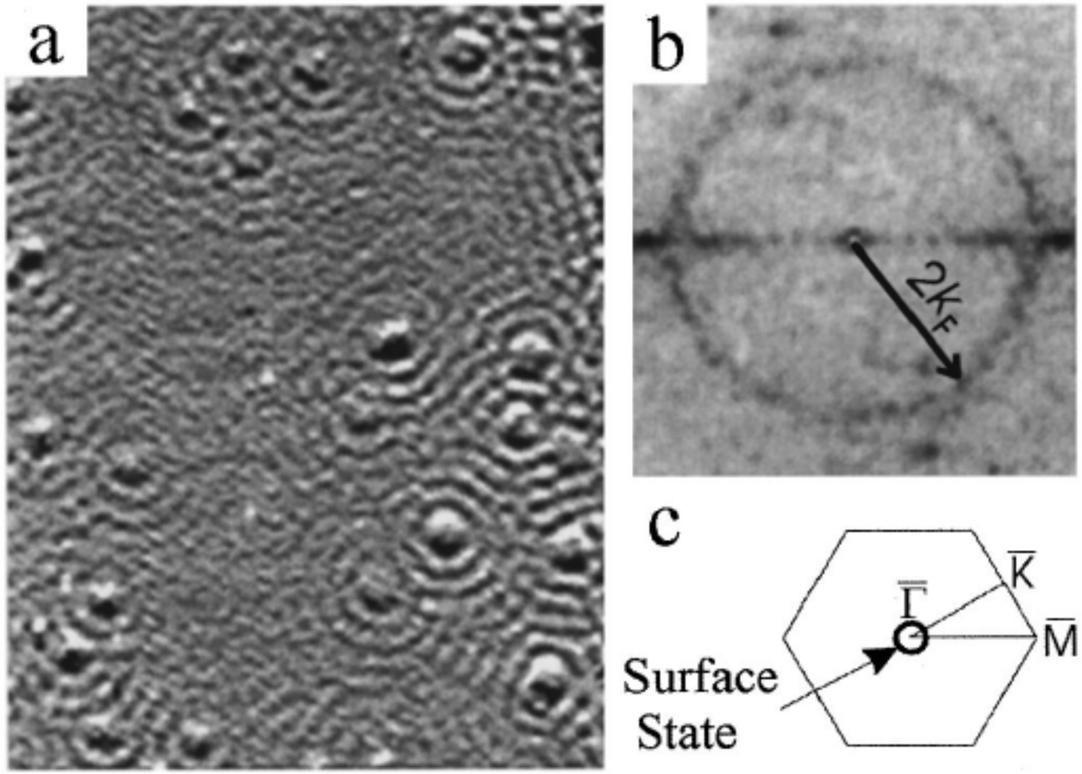
Petersen et al, PRB, 1998



InS(111)

Phys. Rev. Lett. 86 (2001) 3384

Retrieve k-space from STM

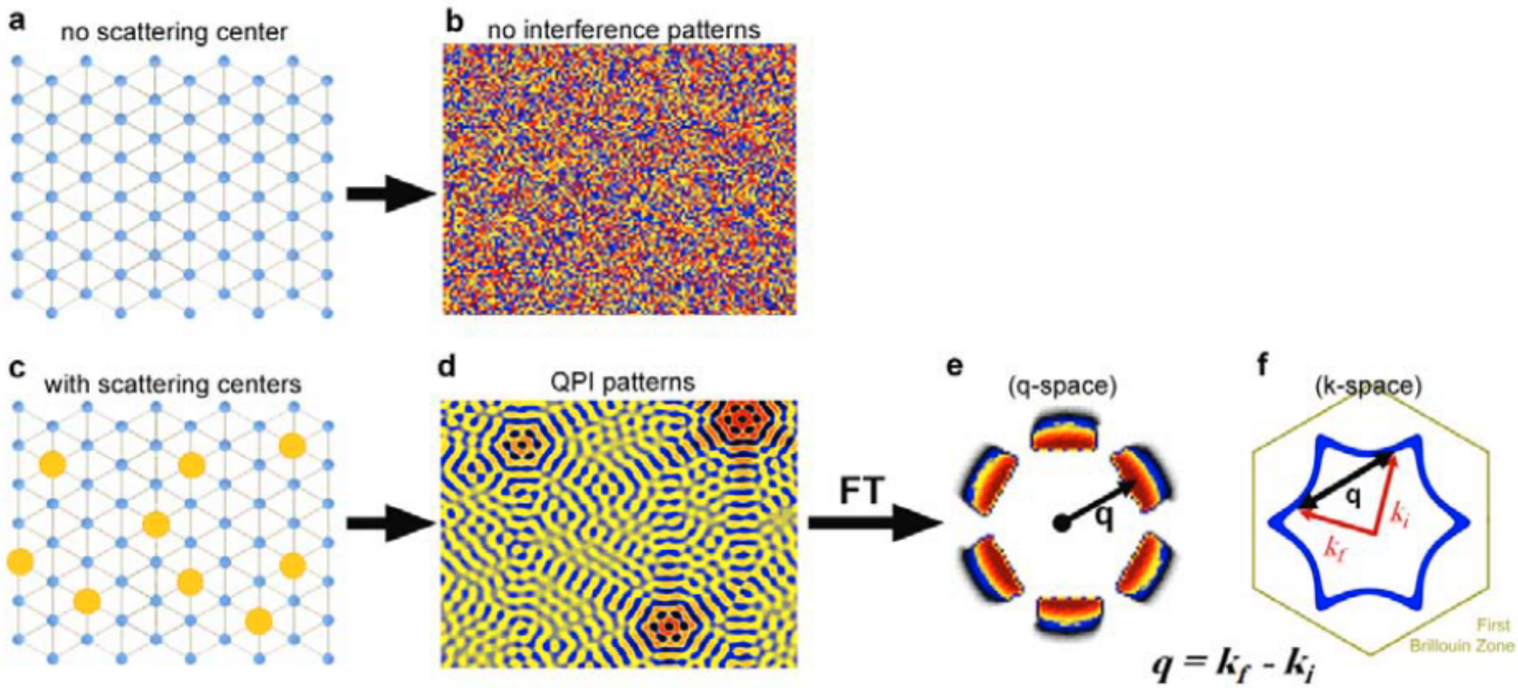


Cu(111)

Petersen et al, PRB, 1998

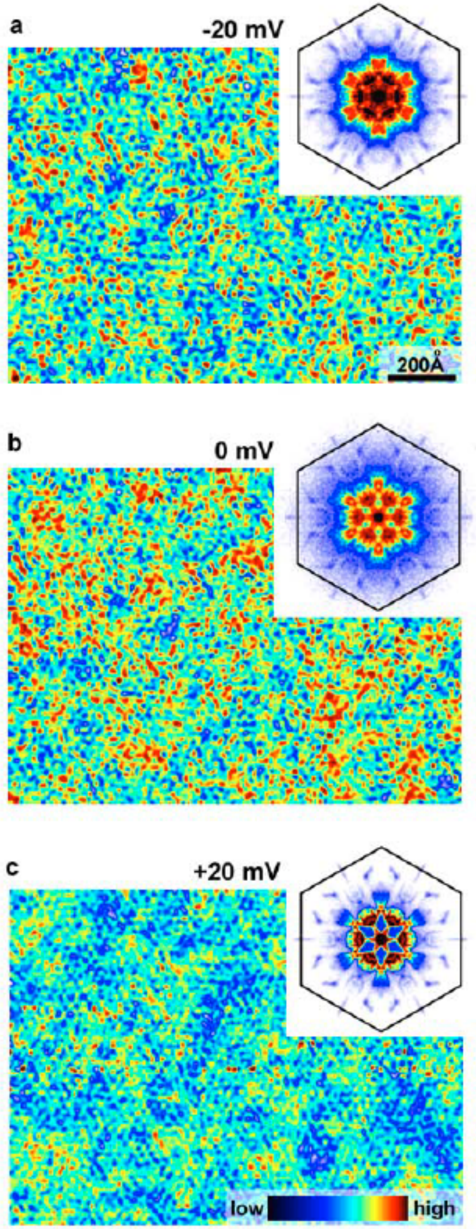
$$\Delta\rho \propto \frac{cos(2k_F + \phi)}{r^2}$$

Mapping TIs

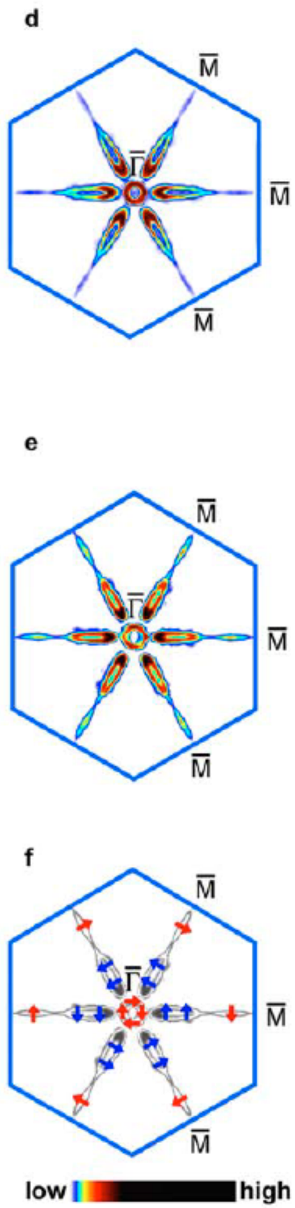


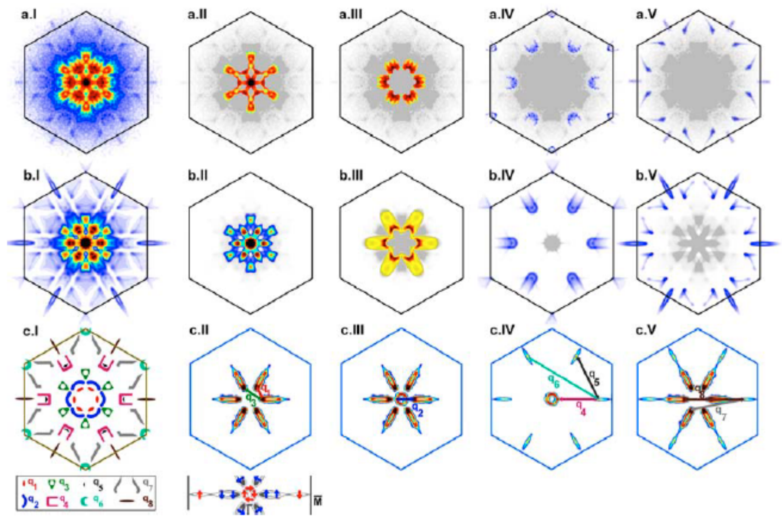
elastic scattering

STM/STS

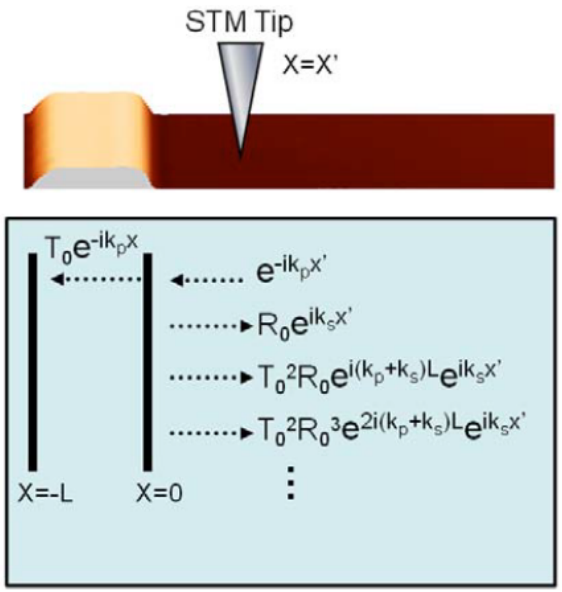


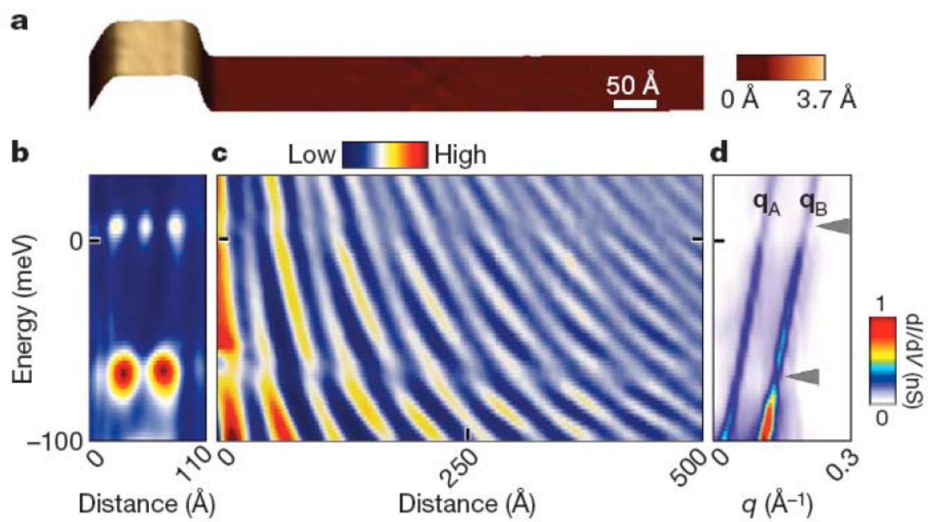
ARPES





Roushan *et al,* Nature, 2009





Seo *et al*, Nature, 2010


Thank You!